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COMPUTER-AIDED DESIGN OF EXPERIMENTS

A THESIS

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TABLE OF CONTENTS

TABLE OF CONTENTS (Concluded)

LIST OF TABLES

LIST OF TABLES (Concluded)

SUMMARY

It is not uncommon that an experiment is decided upon, data are collected, and conclusions are drawn without considering the statistical design of the experiment. It would be advantageous to develop a technique to utilize these undesigned observations while augmenting the experiment with additional observations to enhance the statistical properties of the experiment. The purpose of this investigation is to develop a technique to augment existing undesigned response surface experiments with a limited number of additional observations in such a manner that an appropriate design criterion is optimized. Efforts will be limited to the first order model and the minimum mean square error criterion.

The minimum mean square error criterion cannot be minimized directly because of unknown model parameters; however, this investigation develops an objective function which serves as a criterion that can be minimized. This objective function criterion yields designs with minimum mean square error values close to the most optimal values of minimum mean square error that could be obtained if the model parameters were known. Newton's method for nonlinear systems is used to solve the objective function, and new observations are added to the initial experiment

sequentially.

A statistically weak response surface experimental design may be significantly improved by sequentially adding new observations in the number and manner dictated by the minimization of the objective function. Since the determinant of the ($\underline{X}'\underline{X}$) matrix is generally used in the literature to measure the value of an experimental design, it was computed for all the designs considered in this investigation. The determinant of the ($\underline{X}'\underline{X}$) matrix criterion cannot be considered a valid design criterion in conjunction with the minimization of mean square error.

CHAPTER I

INTRODUCTION

1.1 Repairing Response Surface Designs

It is not uncommon that an experiment is decided upon, data are collected, and conclusions are drawn without considering the statistical design of the experiment. The results of such experiments are often such that important effects are confounded, regression coefficients are biased, or other information is limited in value. Since each measure of the response variable in an experiment represents a commitment of time and resources, such measurements are generally limited. Therefore, it would be advantageous to develop a technique to utilize these undesigned observations while augmenting the experiment with additional observations to enhance the statistical properties of the experiment. Such a technique to "repair" an undesigned experiment should minimize expenses while maximizing the statistical value of the data collected.

Statisticians have long known the value of designed experiments, and certain concepts and techniques have formed a methodology known as design of experiments. Texts by Davies (4), Fisher and Yates (6), Hicks (8) and Kempthorne (9) have documented techniques for designing experiments which are appropriate for most situations. In addition, Box and Wilson (2) have outlined designs to satisfy certain criteria in response surface methodology. Their work has been expanded extensively, culminating in a recent text by Myers (12). All of these techniques assume the experiment is designed in advance of collecting the data, use the method of least squares to estimate model parameters, and usually include an analysis of variance.

Response surface methodology assumes the response can be approximated by a low order polynomial in the independent variables. Usually, a first or second order polynomial model is assumed and the experiment is designed to satisfy some design criterion. If one limits the range of the independent variables to a sufficiently small region, the true response function might have little curvature within this region of interest; and a first order model is often appropriate. In fact, most response surface investigations make an initial first order assumption before a higher order approximation is used. Improper design problems are often found in applying response surface methodology to industrial experimentation. Such designs are generally initiated by experimentors attempting to optimize the response of some system. If the results obtained from such a design are not adequate, a statistician might be asked to repair the experiment within a limited number of additional observations.

1.2 Purpose and Scope

The purpose of this investigation is to develop a technique to augment existing undesigned response surface experiments with a limited number of additional observations in such a manner that an appropriate design criterion is optimized. Efforts will be limited to the first order model and the minimum mean square error criterion. The minimum mean square error is the average of the expected squared deviations of the true response from the estimated response over the design region.

CHAPTER II

LITERATURE REVIEW

Few design repair techniques have been reported in the literature dealing with experimental design. The most extensive approach to the subject is in an unpublished paper by Mitchell (11). Mitchell develops a technique for augmenting a set of existing observations so that the determinant of the $(\underline{X}'\underline{X})$ matrix is maximized. This criterion can be shown to be equivalent to minimizing the variance of the regression coefficients. The technique assumes that the model used to fit the empirical data is correct, and the determinant of the $(\underline{X}'\underline{X})$ matrix criterion offers only limited protection against bias from higher order terms. Assuming an initial matrix $\underline{X}$, Mitchell augments the design with the vectors $a_1, a_2, \ldots, a_m$, to form an augmented matrix $\tilde{\underline{X}}$. That is,

$$\tilde{\underline{X}} = \begin{bmatrix} \underline{X} \\ \hline \underline{A} \end{bmatrix}.$$

Let the ith row of $\underline{A}$ be $\underline{f}(a_i)'$, $i=1, 2, \ldots, m$, and

$$\underline{V} = (\underline{X}'\underline{X})^{-1}, \qquad \tilde{\underline{V}} = (\tilde{\underline{X}}'\tilde{\underline{X}})^{-1}.$$

Using a theorem due to R.L. Plackett (13) one obtains

$$\underline{\tilde{V}}=\underline{V} - \underline{V}\ A'(\underline{I} + \underline{A}\ \underline{V}\ \underline{A}')^{-1}\underline{A}\ \underline{V}, \tag{2.1}$$

and then

$$|\underline{\tilde{V}}| = \frac{|\underline{V}|}{|I + A\ V\ A'|}. \tag{2.2}$$

If only one point is added at a time, that is m=1, and the original design is augmented by the single point a, then A=f(a)'. Substituting into equation (2.1),

$$\underline{\tilde{V}}=\underline{V} - \frac{\underline{V}\ \underline{f}(a)\underline{f}(a)'\underline{V}}{I + \underline{f}(a)'\underline{V}\ \underline{f}\ (a)}$$

and finally

$$|\underline{\tilde{V}}| = \frac{|\underline{V}|}{1 + \underline{f}(a)'\underline{V}\ \underline{f}(a)} \tag{2.3}$$

The determinant of the $(\underline{X}'\underline{X})$ matrix criterion requires minimization of its inverse $|\underline{\tilde{V}}|$. Since the variance of the model parameters equals $\sigma^2(\underline{X}'\underline{X})^{-1}$ or $\sigma^2\underline{V}$, the determinant $|\underline{\tilde{V}}|$ can be minimized in equation (2.3) by placing the augmented point where the variance $\underline{f}(a)'\underline{V}\ \underline{f}(a)$ of the predicted response is greatest.

In summary, Mitchell found that the determinant of ($\underline{X}'\underline{X}$) could be maximized by adding additional points in a sequential fashion at the weakest (in a variance sense) existing place in the design. Adding all M points simultaneously is impractical using Mitchell's method. This investigation will propose an augmentation scheme that uses a different and perhaps more valid criterion for optimality. The proposed method also locates the new observations sequentially.

Another approach is due to Dykstra (5). Dykstra balanced or orthogonalized designs according to three separate criteria. However, each criteria, either directly or indirectly, amounted to maximization of the determinant of the ($\underline{X}'\underline{X}$) matrix. Dykstra recognized that a solution might be obtained by adding one observation at a time; however, he maintained that orthogonality could be guaranteed only by adding new points in pairs. Although orthogonality is not the sole criterion for design optimality in this investigation, it is an important consideration.

Gaylor and Merrill (7) have also considered the augmentation problem and have observed that the maximum variance of a predicted response in an orthogonal design is at one or more of the corners of the experimental region. It was further observed that the variance could be reduced by adding observations at the design corners. These observations were extended to nonorthogonal designs, and it developed that variance could be reduced with a simultaneous move toward orthogonality by adding new points to the corners of the design region. Gaylor and Merrill used the maximization of the determinant of the $(\underline{X}'\underline{X})$ matrix criterion to judge relative improvement in their augmented designs, and they added all M new observations simultaneously. The Gaylor-Merrill technique appears to be the basis for the more explicit development presented by Mitchell. Both techniques, Gaylor-Merrill and Mitchell, suffer the limitations of the $(\underline{X}'\underline{X})$ criterion with regard to protection against bias. In addition, Gaylor and Merrill use orthogonality as the sole consideration in design theory.

Kennard and Stone (10) have considered the slightly related problem of augmenting designs that cannot be bound by a simple geometric shape because of practical limitations. They focus on covering the region of interest by selecting only uniformly spaced observations from an a priori set of candidate points. The technique uses no explicit criterion to measure coverage of the design region but follows a set of general guidelines. The Kennard-Stone technique seems to be applicable only in the special, but certainly practical, situations for which it was developed.

Existing methods of design augmentation in the current literature use, directly or indirectly, the maximization of the determinant of the ($\underline{X}'\underline{X}$) matrix as the optimization criterion. These techniques do not develop explicit objective functions that express this criterion directly. Instead they employ simple search techniques to locate the maximum variance within the design region and add the additional observations at these maximum variance locations. In this investigation a different criterion for optimality, minimum mean square error, which has more intuitive appeal is used. An explicit objective function that expresses this criterion directly will be presented.

CHAPTER III

A PROCEDURE FOR REPAIRING FIRST ORDER RESPONSE SURFACE DESIGNS

3.1 Development of the Mean Square Error Criterion

The goal of this investigation is to develop a technique for augmenting a given, first order, non-optimal design with a limited number of additional observations in such a manner to optimize the design with respect to an appropriate criterion. It is, therefore, necessary to choose a design criterion that not only has intuitive appeal but also lends itself to standard optimization techniques. Most design criteria, such as the determinant of the $(\underline{X}'\underline{X})$ matrix, are directly related to considerations of the variance of the estimated response. These criteria provide only minimal protection against bias of the regression coefficients due to inadequacy of the fitted polynomial. Since in this investigation a first order model is assumed, considerable bias error may be present if the true response function is not linear. Box and Draper (1) have introduced the mean square error criterion which provides a means of considering both bias and variance of the estimated response averaged over the entire region of interest.

In response surface designs a measured response η, a function of k independent variables $\eta=f(x_1,x_2,\ldots,x_k)$, is the experimental data collected. The purpose of an experiment is to estimate the unknown parameters in the function f. These parameters relate the independent variables x_i to the measured response η. The function f is generally approximated by a low order polynomial which in this investigation will be assumed to be first order. That is, the function f is approximated by the polynomial

$$\underline{Y}=\underline{X}\ \underline{\beta} + \underline{\varepsilon}$$

where (ε) is random error assumed to be normally and independently distributed with mean zero and variance σ^2. The $\beta_0,\beta_1,\ldots,\beta_k$ are unknown, constant coefficients of the independent variables x_i and are estimated by the method of least squares. Appendix A contains a development of the least squares estimation of the β_i's. The predicted response is

$$\underline{\hat{Y}}=\underline{X}\ \underline{\hat{\beta}}$$

and in addition

$$\text{Var}\ \underline{\hat{Y}}=\underline{X}'\left[\text{Var}\ \underline{\hat{\beta}}\right]\underline{X}$$

where

$$\text{Var }\hat{\underline{\beta}}=E[\hat{\underline{\beta}}-\underline{\beta}][\hat{\underline{\beta}}-\underline{\beta}]'$$

which reduces to

$$\text{Var }\hat{\underline{\beta}}=\sigma^2(\underline{X}'\underline{X})^{-1} \quad .$$

The mean square error criterion can now be expressed as

$$J=\{[N/\sigma^2]\int_R E[\hat{y}(\underline{x})-f(\underline{x})]^2 d\underline{x}\}/\int_R dx \tag{3.1}$$

where N is the number of observations measured, f is the actual response function, and $\int_R d\underline{x}$ is the volume of the region of interest, R. We see that J is the average of the expected squared deviation of the true response from the estimated response over the region of interest. If one assumes a region of interest R equal to a unit hypersphere, the indicated integration can be easily performed. Appendix B contains the details of the development of J.

An expression may be given for J in terms of the average variance of $\hat{y}$, say V, and the average squared bias of $\hat{y}$, say B. That is,

$$V=1+\sum_{j=1}^{k}(c^{jj}/k+2) \tag{3.2}$$

where c^{jj} is the jjth element of the matrix $\underline{C}=N(\underline{X}'\underline{X})^{-1}$, and

$$B=1/k+2\sum_{g=1}^{k}\{\sum_{i=1}^{k}\sum_{j=i}^{k}\alpha_{ij}\sum_{h=1}^{k}c^{gh}[hij]\}^2 \qquad (3.3)$$

$$+\{\sum_{i=1}^{k}\sum_{j=1}^{k}\alpha_{ij}([ij]-\delta_{ij}/k+2)\}^2$$

$$\frac{+2(k+2)\sum_{i=1}^{k}\alpha_{ii}^2+(k+2)\sum_{i=1}^{k}\sum_{j=i+1}^{k}\alpha_{ij}^2-2(\sum_{i=1}^{k}\alpha_{ii})^2}{(k+2)^2(k+4)}$$

where

$$\alpha_{ij}=\beta_{ij}\sqrt{N}/\sigma, \quad \delta_{ij}=\{\begin{matrix}0 & i\neq j\\ 1 & i=j\end{matrix},$$

and

$$J=V+B.$$

Appendix B also contains a detailed development of equations (3.2) and (3.3).

3.2 Optimization of the Mean Square Error Criterion

The criterion, J, cannot be minimized directly because of the unknown β_{ij}'s; however, it is shown in Appendix C that the average squared bias dominates J. Therefore, if one minimizes bias alone and neglects variance, the resulting design yields values of J very close to the optimal J for designs which assume the β_{ij}'s to be known. It is easily seen from equation (3.3) that the average squared bias B is minimized by forcing all third and mixed second moments of the design matrix to zero, and by forcing all pure second moments to (1/k+2). That is, B is minimized when

$$[hij]=0 \quad \text{or} \quad \sum_{j} \sum_{\ell \geq j}^{k} \sum_{p \geq \ell}^{k} \left(\sum_{i} x_{ij}x_{i\ell}x_{ip}\right)=0 \tag{3.4}$$

$$[ij]=0 \quad \text{or} \quad \sum_{j} \sum_{\ell \geq j}^{k} \left(\sum_{i} x_{ij}x_{i\ell}\right)=0 \tag{3.5}$$

$$[ii]=1/k+1 \quad \text{or} \quad \sum_{j}\left[\sum_{i}(x_{ij}^2)-N/(k+2)\right]=0 \tag{3.6}$$

If the additional restriction that $\sum_{i} x_{ij}=0$ is added, the above requirements can be incorporated into the class of orthogonal designs. The concept of a design moment and the square bracket notation are explained and illustrated in Appendix D. The above conditions, which minimize average squared bias B, can be expressed in a single objective function, say F. That is, B is minimized when F is zero and

$$F(\underline{X})=\sum_{j}\left(\sum_{i} x_{ij}\right)^2+\sum_{j}\left(\sum_{i}(x_{ij}^2)-N/k+2\right)^2 \tag{3.7}$$

$$+\sum_{j} \sum_{\ell \geq j}^{k} \sum_{p \geq \ell}^{k} \left(\sum_{i} x_{ij}x_{i\ell}x_{ip}\right)^2+ \sum_{j} \sum_{j > \ell}^{k} \left(\sum_{i} x_{ij}x_{i\ell}\right)^2.$$

If a set of N experimental trials are given, and M additional observations are allowed to optimize the design, the first N runs will fix the values of x_{ij} for i=1,2,...,N and j=1, 2,...,k. That is, let

$$\sum_{i}^{N} x_{ij}=c_j'$$

$$\sum_{i}^{N} (x_{ij}-N/k+2)=c_j''$$

$$\sum_{i}^{N} (x_{ij}x_{i\ell}x_{ip})=c_{j\ell p}$$

$$\sum_{i}^{N} (x_{ij}x_{i\ell})=c_{j\ell}.$$

The function F can now be written

$$F(\underline{X})=\sum_{j}(c_j'+\sum_{i=N+1}^{M} x_{ij})^2+\sum_{j}(c_j''+\sum_{i=N+1}^{M} x_{ij}^2)^2 \qquad (3.8)$$
$$+\sum_{j}\sum_{\ell\geq j}^{k}\sum_{p\geq j}^{k}(c_{j\ell p}+\sum_{i=N+1}^{M} x_{ij}x_{i\ell}x_{ip})^2+\sum_{j}\sum_{\ell>j}^{k}(c_{j\ell}+\sum_{i=N+1}^{M} x_{ij}x_{i\ell})^2,$$

where the x_{ij} are now only components of the augmented design points.

Numerical techniques may be used to minimize the function F. Newton's method is used in this investigation and adequate results are obtained. However, reduced computing time and greater generality might be obtained by using more sophisticated methods for solving non-linear systems. Using Newton's method, the first partial derivatives of equation (3.8) with respect to each of the variables x_{ij} are required. It is convenient to limit M to one and add new observations sequentially, therefore

$$\frac{\partial F(\underline{X})}{\partial x_{11}} = {}_{11}f = 2(c_1'+x_{11})+2(c_1''+x_{11}^2)2x_{11} \tag{3.9}$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[(c_{1p\ell}+x_{11}x_{1\ell}x_{1p})\frac{\partial(x_{11}x_{1\ell}x_{1p})}{\partial x_{11}}\right]$$

$$+2\sum_{\ell=2}^{k}(c_{1\ell}+x_{11}x_{1\ell})x_{1\ell}$$

$$\frac{\partial F(\underline{X})}{\partial x_{12}} = {}_{12}f = 2(c_1'+x_{12})+2(c_1''+x_{12}^2)2x_{12} \tag{3.10}$$

$$+2\sum_{\ell\geq 2}^{k}\sum_{p\geq \ell}^{k}\left[(c_{2p\ell}+x_{12}x_{1\ell}x_{1p})\frac{\partial(x_{12}x_{1\ell}x_{1p})}{\partial x_{12}}\right]$$

$$+2\sum_{\ell=3}^{k}(c_{1\ell}+x_{12}x_{1\ell})x_{1\ell}$$

$$\vdots \qquad\qquad\qquad \vdots$$

$$\frac{\partial F(\underline{X})}{\partial x_{1j}} = {}_{1j}f = 2(c_j' + x_{1j}) + 2(c_j'' + x_{1j}^2)2x_{1j} \tag{3.11}$$

$$+2\sum_{\ell \geq j}^{k}\sum_{p \geq \ell}^{k}\left[(c_{jp\ell} + x_{1j}x_{1\ell}x_{1p})\frac{\partial(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}}\right]$$

$$+2\sum_{\ell > j}^{k}(c_{j\ell} + x_{1j}x_{1\ell})x_{1\ell}\ .$$

In addition, second partial derivatives of equations (3.9) through (3.11) with respect to all variables x_{ij} are required. That is,

$$\frac{\partial^2 F(\underline{X})}{\partial x_{11}^2} = {}_{11}f_{11} = 2 + 4\left[(c_1'' + x_{11}^2) + 2x_{11}^2\right] + 2\sum_{\ell=2}^{k} x_{1\ell}^2$$

$$+2\sum_{\ell \geq 1}^{k}\sum_{p \geq \ell}^{k}\left[\left(\frac{\partial(x_{11}x_{1\ell}x_{1p})}{\partial x_{11}}\right)^2 + (c_{1p\ell} + x_{11}x_{1\ell}x_{1p})\frac{\partial^2(x_{11}x_{1\ell}x_{1p})}{\partial x_{11}^2}\right]$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{11}\partial x_{12}} = {}_{11}f_{12} = 2(c_{12} + x_{11}x_{12}) + 2x_{12}x_{11} +$$

$$+2\sum_{\ell \geq 1}^{k}\sum_{p \geq \ell}^{k}\left[\frac{\partial(x_{11}x_{1\ell}x_{1p})}{\partial x_{12}}\ \frac{\partial(x_{11}x_{1\ell}x_{1p})}{\partial x_{11}} + \right.$$

$$\left.(c_{1p\ell} + x_{11}x_{1\ell}x_{1p})\frac{\partial^2(x_{11}x_{1\ell}x_{1p})}{\partial x_{11}\partial x_{12}}\right]$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{11}\partial x_{1j}} = {}_{11}f_{1j} = 2(c_{1j}+x_{11}x_{1j})+2x_{11}x_{1j}$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\frac{\partial(x_{11}x_{1\ell}x_{1p})}{\partial x_{1j}}\;\frac{\partial^2(x_{11}x_{1\ell}x_{1p})+}{\partial x_{11}\partial x_{1j}}\right.$$

$$\left.(c_{1p\ell}+x_{11}x_{1\ell}x_{1p})\frac{\partial^2(x_{11}x_{1\ell}x_{1p})}{\partial x_{11}\partial x_{1j}}\right]$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{12}\partial x_{11}} = {}_{12}f_{11} = 2(c_{12}+x_{11}x_{12})+2x_{12}x_{11}+$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\frac{\partial(x_{12}x_{1\ell}x_{1p})}{\partial x_{11}}\;\frac{\partial(x_{12}x_{1\ell}x_{1p})+}{\partial x_{12}}\right.$$

$$\left.(c_{2p\ell}+x_{12}x_{1\ell}x_{1p})\frac{\partial^2(x_{12}x_{1\ell}x_{1p})}{\partial x_{12}\partial x_{11}}\right]$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{12}^2} = {}_{12}f_{12} = 2+4\left[(c_2''+x_{12}^2)+2x_{12}\right]+2\sum_{\ell=3}^{k}x_{1\ell}^2$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\left(\frac{\partial(x_{12}x_{1\ell}x_{1p})}{\partial x_{12}}\right)^2+(c_{2p\ell}+x_{12}x_{1\ell}x_{1p})\right.$$

$$\left.\cdot\;\frac{(\partial^2(x_{12}x_{1\ell}x_{1p}))}{\partial x_{12}^2}\right]$$

$$\vdots \qquad\qquad\qquad\qquad \vdots$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{12}\partial x_{1j}} = {}_{12}f_{1j} = 2(c_{1j}+x_{12}x_{1j})+2x_{12}x_{1j}$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\frac{\partial(x_{12}x_{1\ell}x_{1p})}{\partial x_{12}}\ \frac{\partial(x_{12}x_{1\ell}x_{1p})}{\partial x_{1j}} + (c_{2p\ell}+x_{12}x_{1\ell}x_{1p})\frac{\partial^2(x_{12}x_{1\ell}x_{1p})}{\partial x_{12}\partial x_{1j}}\right]$$

$$\vdots \qquad\qquad \vdots$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{1j}\partial x_{11}} = {}_{1j}f_{11} = 2(c_{1j}+x_{11}x_{1j})+2x_{11}x_{1j}$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\frac{\partial(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}}\ \frac{\partial(x_{1j}x_{1\ell}x_{1p})}{\partial_{11}} + (c_{jp\ell}+x_{1j}x_{1\ell}x_{1p})\frac{\partial^2(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}\partial x_{11}}\right]$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{1j}\partial x_{12}} = {}_{1j}f_{12} = 2(c_{1j}+x_{1j}x_{12})+2x_{12}x_{1j}$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\frac{\partial(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}}\ \frac{\partial(x_{1j}x_{1\ell}x_{1p})}{\partial x_{12}} + (c_{jp\ell}+x_{1j}x_{1\ell}x_{1p})\frac{\partial^2(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}\partial x_{12}}\right]$$

$$\vdots \qquad\qquad \vdots$$

$$\frac{\partial^2 F(\underline{X})}{\partial x_{1j}^{\,2}} = {}_{1j}f_{1j} = 2+4\left[(c_j'' + x_{1j}^2) + 2x_{1j}^2\right] + 2\sum_{\ell>j}^{k} x_{1\ell}^2$$

$$+2\sum_{\ell\geq 1}^{k}\sum_{p\geq \ell}^{k}\left[\left(\frac{\partial(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}}\right)^2 + (c_{jp\ell} + x_{1j}x_{1\ell}x_{1p})\frac{\partial^2(x_{1j}x_{1\ell}x_{1p})}{\partial x_{1j}^{\,2}}\right].$$

The minimum of $F(\underline{X})$ is now found through the iterative equation

$$x_{gh} - x_{gh}^0 = \frac{\begin{vmatrix} {}_{11}f_{11} & {}_{12}f_{11} & \cdots & {}_{11}f & \cdots & {}_{1j}f_{11} \\ {}_{11}f_{12} & {}_{12}f_{12} & \cdots & {}_{12}f & \cdots & {}_{1j}f_{12} \\ \vdots & \vdots & & & & \vdots \\ {}_{11}f_{1j} & {}_{12}f_{1j} & \cdots & {}_{1j}f & \cdots & {}_{1j}f_{1j} \end{vmatrix}}{\begin{vmatrix} {}_{11}f_{11} & {}_{12}f_{11} & \cdots & {}_{gh}f_{11} & \cdots & {}_{1j}f_{11} \\ {}_{11}f_{12} & {}_{12}f_{12} & \cdots & {}_{gh}f_{12} & \cdots & {}_{1j}f_{12} \\ \vdots & \vdots & & \vdots & & \vdots \\ {}_{11}f_{1j} & {}_{12}f_{1j} & \cdots & {}_{gh}f_{1j} & \cdots & {}_{1j}f_{1j} \end{vmatrix}} \qquad (3.12)$$

where x_{gh} represents a specific variable x_{ij} and x_{gh}^o represents an initial starting estimate for the iterative procedure. The denominator of equation (3.12) is the Jacobian of the functions $({}_{11}f, {}_{12}f, \ldots, {}_{1j}f)$, and the vector

$({}_{11}f, {}_{12}f, \ldots, {}_{1j}f)'$ replaces the vector $({}_{gh}f_{11}, {}_{gh}f_{12}, \ldots, {}_{gh}f_{1j})'$ in the Jacobian to form the numberator of equation (3.12).

Using Newton's method the necessary conditions for a minimal solution to the objective F are satisfied; however, sufficiency is not satisfied. The third partial derivatives of the objective function would provide the sufficiency requirement; but this method would unduly lengthen computing time. It is adequate to observe the successive values of F and judge sufficiency if F moves toward a minimum value during the iterative solution process. Newton's method will converge if the initial estimate of the solution is sufficiently close to the final solution. However, it is very difficult to estimate the x_{ij}'s for more than one observation at a time. For this reason M was limited to one and the observations were added sequentially. If one examines an all-bias design (12), it is seen that the design is perfectly balanced with respect to orthogonality and location of design points about the center of the region of interest. In addition all x_{ij} are located at

$$G=\pm\sqrt{1/(k+2)}\ .$$

These facts lead to an iterative scheme for producing initial estimates of the additional observations which are sufficient for Newton's method to converge quickly. If each point in the design matrix is considered a vector in the space defined by the region of interest, the resultant vector of all vectors or design points in a perfectly designed experiment is zero. The augmented design point is, therefore, selected to force the resultant vector of the augmented design matrix to zero, and it is simultaneously clustered about G. Appendix E contains an example estimate of an initial design point.

A procedure for selecting an appropriate design criterion, and a method for optimizing that criterion have been discussed. It remains to develop some control criteria to give one a measure of design improvement using the above augmentation procedures. It is natural to consider the determinant of the $(\underline{X}'\underline{X})$ matrix because of its nearly universal use in the literature. In addition, values for V, B, and J may be estimated if one assumes certain values for the β_{ij}'s and σ^2. In this investigation the β_{ij}'s are all chosen to be one and σ is chosen to be 0.1, 0.2, and 0.05. A ratio of improvement that compares J for the initial undesigned experiment, say J_I, to J for the final augmented design, say J_F, can also be computed. Since J is a function of the number of observations N, a correction factor for J_I and J_F must be applied. The J value for a perfectly designed all-bias experiment of the same design dimensions as the undesigned experiment, say J_{ABI}, is subtracted from J_I, and in similar fashion J for a designed all-bias experiment of the same dimensions as the final augmented experiment, say J_{ABF}, is subtracted from J_F. Now the improvement ratio may be expressed as

$$IR = \frac{J_F - J_{ABF}}{J_I - J_{ABI}} ,$$

which tends to zero as the final augmented design approaches the designed all-bias experiment. Finally, the value of the objective function F(X) can be compared before and after augmentation. All of the above criteria are computed for each design considered. Appendix C contains tables of these criteria by design dimensions.

To test the proposed procedure, near random designs are generated through a modification of the subroutine, RANDU (14), and they are used as the assumed undesigned experiments to be optimized. Undesigned experiments consisting of two independent variables with four, five, and eight runs and three independent variables with six, eight and ten runs, are considered. The number of augmented observations for each test case design begins with one and is increased sequentially to the required number of additional observations. Each experimental design (arrangement of N, k, and M) is replicated (10) times. The FORTRAN program used in this investigation is reproduced in Appendix F.

CHAPTER IV

DISCUSSION OF RESULTS

The objective of this investigation was to develop a procedure for repairing inadequate response surface designs by augmenting them with additional observations. Improvement in the repaired designs was to be measured by the relative minimization of average squared bias B. The average squared bias was minimized by minimizing an objective function $F(\underline{X})$. If a statistician is allowed M additional observations to repair a design, he might use the technique developed in this investigation to tabulate the value of $F(\underline{X})$ for each additional observation sequentially and then pick a number of new experimental observations that corresponds to the minimum value of $F(\underline{X})$.

The results of this investigation are detailed for each experimental design considered in Appendix C. The minimum value for the minimization function $F(\underline{X})$ does not always correspond to the minimum value of average squared bias B as was expected. However, recalling the discussion of the repair problem in Chapter I, it was asserted that design repair is required when an initial design produces inadequate results. Since, in this investigation, initial designs were chosen by a random process, it is not unlikely that some random placing of observations might evenly cover the region of interest and, thereby produce a near optimal design. It also seems likely that as the number of observations increase relative to the number of independent variables, the probability of improving the coverage of the region of interest will increase. In fact, the results of this investigation tabulated in Appendix C verify these conjectures. Since the design repair technique in this investigation was envisioned for use on poor initial designs, it is reasonable to disregard those designs which are initially optimal with respect to average squared bias. Designs which are initially near-optimal with respect to average squared bias, that is the initial value of B is of the same order of magnitude as the minimum value of B, may also yield poor results.

The value of $F(\underline{X})$ as a predictor of the average squared bias can be tabulated. Consider any given experimental design for which new observations are added sequentially, let the initial value for B be B_o, the minimum value of B be B_m, and the value of B that corresponds to the minimum value of the minimization function $F(\underline{X})$ be B_f. Then the percentage bias loss incurred by choosing M to correspond to the minimum value of $F(\underline{X})$ can be estimated as

$$PBL = \frac{(B_o-B_m)-(B_o-B_f)}{(B_o-B_m)} \times 100\%$$

Values of PBL are tabulated in Tables 1 and 2. Designs which were optimal with respect to average squared bias in the initial case are disregarded, and near optimal initial designs are noted by an asterik.

Since average squared bias and minimum mean square error cannot be minimized directly, the objective function F is minimized by the sequential addition of new experimental observations. The minimum value of the F criterion provides a new augmented design which is close to a design that would be obtained if B and J could be minimized directly. Several designs are not satisfactorily improved by the minimization of $F(\underline{X})$. Most of these anomalies are either nearly optimal in the initial design and are noted by an asterisk, or the initial design values of B are of the same order of magnitude as the optimal design values of B.

The determinant of the $(\underline{X}'\underline{X})$ matrix is tabulated for each design considered in this investigation. In addition the determinant of the $(\underline{X}'\underline{X})$ matrix is computed for each new observation added to a given design. The results of this investigation indicate a monotonic increase in this criterion with each additional observation. In fact, this criterion continued to increase when the average squared bias reached very large, unacceptable values. For example, consider test case 4 of experimental design N=10, k=3,

Table 1. Values of Percentage Bias Loss

Experimental Designs with Two Independent Variables

Design / Test Case	N=4, k=2 M=4	N=5, k=2 M=5	N=8, k=2 M=5
1	3.84%	17.46%	
2	.19	11.81	79.49%*
3	0	66.95	207.08 *
4	0	.68	
5	.76	15.36	
6			176.09 *
7	4.51		
8	1.59	38.64	8.64
9	2.36	56.67	44.47
10	.68		

Table 2. Values of Percentage Bias Loss

Experimental Designs with Three Independent Variables

Design / Test Case	N=6, k=3 M=4	N=8, k=3 M=5	N=10, k=3 M=7
1	.62%	0 %	2.58%
2	0	11.49	15.92
3	61.83	1.59	1.77
4	20.24	4.98	0
5	0	3.42	0
6	10.55	1.44	4.14
7	1.37	1.97	24.22
8	1.90	0	0
9	0	8.80	23.02
10	0	57.60	11.66

and M=7. This example shows that the determinant of the ($\underline{X}'\underline{X}$) matrix increased from a low of 3.774 to a high of 40,393.281 in seven steps while the average squared bias began at 10,317.319, dropped to a low of 1678.968, and rose to a high of 423,674.965. The determinant of the ($\underline{X}'\underline{X}$) matrix typically reflected none of these fluctuations in B. If the minimum mean square error criterion is accepted, the determinant of the ($\underline{X}'\underline{X}$) matrix criterion seems to be invalid.

Average squared bias was assumed to dominate the minimum mean square error in the development of the objective function F($\underline{X}$). The results of this investigation justify this assumption. However, the degree of domination of B over J is determined by the β_{ij}/σ ratio. As reflected by the tables in Appendix C, the domination of B over J is more pronounced as the ratio β_{ij}/σ is increased. It is conceivable that the ratio of model parameters to σ could be sufficiently decreased to negate this dominance and invalidate the all-bias criterion. All ratios of β_{ij}/σ in this investigation are sufficiently large to guarantee the dominance of B over J. The computed values of minimum mean square error and improvement ratio, therefore, afford no additional insight into the relative improvement of any given design augmentation.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS FOR FURTHER STUDY

5.1 Conclusions

Three significant conclusions are indicated by the results of this investigation. They are, in order of importance:

1. An undesigned, statistically weak response surface experiment may be significantly improved by sequentially adding new observations in the number and manner dictated by the minimization of the function $F(\underline{X})$ which yields designs with J values close to the optimal values of J.
2. The determinant of the $(\underline{X}'\underline{X})$ matrix criterion cannot be considered a valid design criterion in conjunction with the minimization of mean square error.
3. The assumption that minimum mean square error is dominated by average squared bias is valid only so long as the ratio of model parameters to σ is sufficiently large.

5.1 Recommendations for Further Study

Several important areas were not considered in this investigation and merit additional study. It would seem desirable to add all additional observations simultaneously. Such a simultaneous augmentation technique could provide greater flexibility in the selection of the additional observations and thereby further reduce the optimal value of the objective function $F(\underline{X})$. However, as previously stated, it is extremely difficult to estimate an initial solution for more than one observation at a time. If an estimation technique for multiple initial observations could be developed, simultaneous augmentation of all new observations would be possible.

The data produced in this investigation suggests that all terms of equation (3.3) are not of equal weight when minimizing the average squared bias. However, the relative importance of any one of the terms of equation (3.3) compared to the other terms if not always constant. If it could be shown that the average squared bias is dominated by a specific term in equation (3.3) for a given range of observations, minimization of B could be simplified by concentrating on this term.

Since the results of this investigation indicated that statistically weak, first order designs could be improved by the augmentation technique presented, it would be desirable to extend the technique to the second order case. Certain design parameters that minimize minimum mean square error for second order rotatable designs have been tabulated by Box and Draper (2). It remains to develop an objective function $F(\underline{X})$ which can be minimized and simultaneously minimizes mean square error.

A block effect introduced by time delays is potentially present in any augmented design. This block effect has not been considered in this investigation. However, adding an additional, dummy independent variable at the zero level to the initial experimental designs would allow the statistician to isolate the blocking effect in the augmented designs and measure its importance. It would be informative to sequentially decrease the β_{ij}/σ ratio to determine an explicit meaning for the statement that average squared bias dominates minimum mean square error if the ratio is sufficiently large. Since the augmentation technique developed in this investigation seems most effective when the initial experimental design is very poor, it would be advisable to assemble a number of practical response surface designs that need repair and measure the value of this augmentation technique on these real world problems.

Finally, this investigation casts doubt on the validity of the determinant of the $(\underline{X}'\underline{X})$ matric criterion. Since this criterion has near universal use in the literature, it would be valuable to study further the relationship between the determinant of the $(\underline{X}'\underline{X})$ matrix and minimum mean square error.

APPENDIX A

LEAST SQUARES METHOD OF ESTIMATION

Given the model

$$\underline{Y}=\underline{X}\ \underline{\beta} + \underline{\varepsilon}$$

where

$$\underline{Y}=\begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_N \end{bmatrix}, \quad \underline{\beta}=\begin{bmatrix} \beta_0 \\ \beta_1 \\ \cdot \\ \cdot \\ \cdot \\ \beta_k \end{bmatrix}, \quad \underline{\varepsilon}=\begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \cdot \\ \cdot \\ \cdot \\ \varepsilon_N \end{bmatrix}$$

and

$$\underline{X}=\begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1k} \\ 1 & x_{21} & x_{22} & & x_{2k} \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ \cdot & \cdot & \cdot & & \cdot \\ 1 & x_{N1} & x_{N2} & & x_{Nk} \end{bmatrix}$$

Let

$$\underline{L}=\sum_{i=1}^{N} \varepsilon_i{}^2=\underline{\varepsilon}'\underline{\varepsilon}$$

Minimizing L, therefore, minimizes the sum of squares error. L can be expressed as

$$\underline{L}=(\underline{Y}-\underline{X}\ \underline{\beta})'(\underline{Y}-\underline{X}\ \underline{\beta})$$

$$L=\underline{Y}'\underline{Y}-(\underline{X}\ \underline{\beta})'\underline{Y}-\underline{Y}'\underline{X}\ \underline{\beta}+(\underline{X}\ \underline{\beta})'\underline{X}\ \underline{\beta}$$

$$L=\underline{Y}'\underline{Y}-\underline{\beta}'\underline{X}'\underline{Y}-\underline{Y}'\underline{X}\ \underline{\beta}+\underline{\beta}'\underline{X}'\underline{X}\ \underline{\beta}$$

$$L=\underline{Y}'\underline{Y}-2\underline{\beta}'\underline{X}'\underline{Y}+\underline{\beta}'\underline{X}'\underline{X}\ \underline{\beta}.$$

The β which minimizes L is found by

$$\frac{\partial L}{\partial \beta}=-2\underline{X}'\underline{Y}+2(\underline{X}'\underline{X})\underline{\hat{\beta}}=0$$

$$(\underline{X}'\underline{X})\underline{\beta}=\underline{X}'\underline{Y}$$

$$\underline{\hat{\beta}}=(\underline{X}'\underline{X})^{-1}\underline{X}'\underline{Y} \tag{A.1}$$

Equation (A.1) is the least squares estimator of the model parameters β_{ij}.

APPENDIX B

DEVELOPMENT OF THE MINIMUM MEAN SQUARE ERROR CRITERION

Consider an assumed experimental design model of order δ_1 with k independent variables. If the true model is of order δ_2 greater than δ_1, then we have a predicted response $\hat{y}(x_1,x_2,\ldots,x_k)$ with degree δ_1, and the true response is $g(x_1,x_2,\ldots,x_k)$ with degree δ_2.

The mean square error is defined to be the expected value of error squared, that is

$$E\left[\hat{y}(x_1,x_2,\ldots,x_k)-g(x_1,x_2,\ldots,x_k)\right]^2$$

which may be written

$$E\left[\hat{y}-g\right]^2 .$$

Let $\int_R d\underline{x}$ be the volume of the region of interest, then the J criterion is defined to be

$$J=N/\sigma^2\left[\frac{\int_R E\left[\hat{y}-g\right]^2 d\underline{x}}{\int_R d\underline{x}}\right] . \tag{B.1}$$

Let

$$K=1/\int_R d\underline{x}$$

$$J=NK/\sigma^2\int_R E\left[\hat{y}-g\right]^2 d\underline{x}$$

$$J=NK/\sigma^2\int_R E\left[\hat{y}^2-2\hat{y}g+g^2\right] d\underline{x}$$

$$J=NK/\sigma^2\int_R E\left[\hat{y}^2-2\hat{y}g+g^2+E\left[\hat{y}\right]^2-E\left[\hat{y}\right]^2\right] d\underline{x}$$

$$J=NK/\sigma^2\int_R \left[\{E\left[\hat{y}^2\right]-E\left[\hat{y}\right]^2\}+\{E\left[\hat{y}\right]^2-2gE\left[\hat{y}\right]+g^2\}\right] d\underline{x}$$

$$J=NK/\sigma^2\int_R E\left[\hat{y}-E\left[\hat{y}\right]\right]^2 d\underline{x} + NK/\sigma^2\int_R \left[E\left[\hat{y}\right]-g\right]^2 d\underline{x} \ ,$$

and

$$J=V+B$$

where

$$V=NK/\sigma^2\int_R E\left[\hat{y}-E\left[\hat{y}\right]\right]^2 d\underline{x} \qquad (B.2)$$

and

$$B=NK/\sigma^2\int_R \left[E\left[\hat{y}\right]-g\right]^2 d\underline{x} \qquad (B.3)$$

since

$$\text{Var } (\hat{y}) = E\left[\hat{y} - E[\hat{y}]\right]^2$$

$$\text{Var } (\hat{y}) = \text{Var } (\underline{x}'\underline{\hat{\beta}})$$

$$= \underline{x}' \text{ Var}(\hat{\beta}_1)\underline{x}$$

$$= \sigma^2 \underline{x}'(\underline{x}'\underline{x})^{-1}\underline{x}$$

substituting into equation (B.2)

$$V = NK/\sigma^2 \int_R \sigma^2 \underline{x}'(\underline{x}'\underline{x})^{-1}\underline{x}$$

$$V = NK \int_R \underline{x}'(\underline{x}'\underline{x})^{-1}\underline{x} \quad . \qquad \text{(B.4)}$$

Let δ_1 be one, then $\hat{y}$ is a first order response and may be written

$$\hat{y} = \underline{x}_1{}'\underline{\hat{\beta}}_1$$

It follows that δ_2 is greater than one, and g is of higher order than one and can be written

$$g = \underline{x}_1'\underline{\beta}_1 + \underline{x}_2'\underline{\beta}_2 + \varepsilon$$

where the term $\underline{x}_2'\beta_2$ represents those higher order terms not included in

$$\hat{y}=\underline{x}_1\hat{\underline{\beta}}_1 \quad .$$

The bias of the element $\hat{\underline{\beta}}_1$, is

$$E(\hat{\underline{\beta}}_1) = \underline{\beta}_1 + \underline{A}\ \underline{\beta}_2 \ .$$

where $\underline{A}$ is the alias matrix as defined by Myers (12). Then

$$E(\hat{y})=E(\underline{x}_1'\hat{\underline{\beta}}_1)$$

$$=\underline{x}_1'E(\hat{\underline{\beta}}_1)$$

$$=\underline{x}_1'(\underline{\beta}_1+\underline{A}\ \underline{\beta}_2)$$

$$E(\hat{y})-g=\underline{x}_1'(\underline{\beta}_1+\underline{A}\ \underline{\beta}_2)-(\underline{x}_1'\underline{\beta}_1+\underline{x}_2'\underline{\beta}_2)$$

$$=\underline{x}_1'\underline{A}\ \underline{\beta}_2-\underline{x}_2'\underline{\beta}_2 \quad .$$

Substituting into equation (B.3)

$$B=NK/\sigma^2\int_R(\underline{x}_1'\underline{A}\ \underline{\beta}_2-\underline{x}_2'\underline{\beta}_2)^2d\underline{x}$$

$$B=NK/\sigma^2\int_R\underline{\beta}_2'(\underline{A}'\underline{x}_1-\underline{x}_2)(\underline{x}_1'\underline{A}-\underline{x}_2')\underline{\beta}_2d\underline{x} \tag{B.5}$$

Let the region of interest R be an unit hypersphere, that is

$$\sum_{i=1}^{k} x_i^2 \leq 1$$

and let

$$\delta_1=1, \quad \delta_2=2$$

then equations (B.4) and (B.5) require evaluation of integrals of the form

$$\int_R x_1^{\delta_1} x_2^{\delta_2} \ldots x_k^{\delta_k} d\underline{x} \quad .$$

It can be shown that

$$\int_R x_1^{\delta_1} x_2^{\delta_2} \ldots x_k^{\delta_k} d\underline{x} = \begin{cases} 0 & \text{if any } \delta_i \text{ is odd} \\ \dfrac{\Gamma\left(\frac{\delta_1+1}{2}\right)\Gamma\left(\frac{\delta_2+1}{2}\right)\ldots\Gamma\left(\frac{\delta_k+1}{2}\right)}{\Gamma\left(\sum_{i=1}^{k}\frac{\delta_i+1}{2}+1\right)} & \text{for all } \delta_i \text{ even .} \end{cases} \tag{B.6}$$

Consider V as expressed in equation (B.4),

$$V/K=N\int_R \underline{x}_1'(\underline{x}_1'\underline{x}_1')^{-1}\underline{x}_1 d\underline{x}$$

$$=\int_R \sum_{i=0}^{k} \sum_{j=0}^{k} x_i x_j c^{ij} d\underline{x}$$

where c^{ij} is an element of the precision matrix

$$\underline{C}=N(\underline{X}'\underline{X})^{-1}.$$

Then

$$V/K=\sum_{i=0}^{k}\ \sum_{j=0}^{k} c^{ij}\int_R x_i x_j d\underline{x}\quad .$$

Now from equation (B.6)

$$\int_R x_i x_j d\underline{x}=0 \qquad \text{if } i\neq j$$

and

$$V/K=\sum_{i=0}^{k} c^{ii}\int_R x_i^2 d\underline{x} \quad \text{if } i=j. \tag{B.7}$$

Again from equation (B.6)

$$K^{-1}=\int_R d\underline{x}$$

$$=\frac{[\Gamma(1/2)]^k}{\Gamma(k/2+1)}$$

$$=\frac{(\pi)^{k/2}}{k/2\Gamma(k/2)}$$

$$\int_R x_i^2 d\underline{x} = \frac{\Gamma(3/2)\Gamma(1/2)\ldots\Gamma(1/2)}{\Gamma(\frac{k+2}{2}+1)}$$

$$= \frac{1/2(\pi)^{k/2}}{(\frac{k+2}{2})\Gamma(\frac{k+2}{2})}$$

$$= \frac{(\pi)^{k/2}}{(k+2)\Gamma(\frac{k+2}{2})} \quad .$$

Substituting into equation (B.7)

$$V = \frac{\sum_{i=0}^{k} c^{ii} \dfrac{(\pi)^{k/2}}{(k+2)\Gamma(\frac{k+2}{2})}}{\dfrac{(\pi)^{k/2}}{k/2\,\Gamma(k/2)}}$$

$$V = 1 + \left(\sum_{i=0}^{k} c^{ii}\right)\left(\frac{1}{k+2}\right)$$

$$V = 1 + \frac{1}{k+2}\left(\sum_{i=0}^{k} c^{ii}\right) \tag{B.8}$$

The integrated squared bias is written in equation (B.5) as

$$B = NK/\sigma^2 \int_R \underline{\beta}_2'(\underline{A}'\underline{x}_1 - \underline{x}_2)(\underline{x}_1'\underline{A} - \underline{x}_2')\underline{\beta}_2 d\underline{x} \quad .$$

Let

$$\alpha_2=\underline{\beta}_2\sqrt{N}/\sigma$$

then

$$B/K=\alpha_2'\underline{A}'(\int_R \underline{x}_1\underline{x}_1'd\underline{x})\underline{A}\alpha_2-2\alpha_2-2\alpha_2'(\int_R \underline{x}_2\underline{x}_1'd\underline{x})\underline{A}\alpha_2+\alpha_2'(\int_R \underline{x}_2\underline{x}_2'd\underline{x})\alpha_2$$

$$B=\alpha_2'\underline{A}'(K\int_R \underline{x}_1\underline{x}_1'd\underline{x})\underline{A}\alpha_2-2\alpha_2'(K\int_R \underline{x}_2\underline{x}_1'd\underline{x})\underline{A}\alpha_2 \tag{B.9}$$

$$+\alpha_2'(K\int_R\underline{x}_2\underline{x}_2'd\underline{x})\alpha_2 \ .$$

Consider the matrix

$$K\int_R \underline{x}_1\underline{x}_1'd\underline{x}$$

that is

$$\begin{bmatrix} K\int_R 1d\underline{x} & 0 & 0 & \cdots & 0 \\ 0 & K\int_R \underline{x}_1^2d\underline{x} & 0 & \cdots & 0 \\ 0 & 0 & K\int_R \underline{x}_2^2d\underline{x} & \cdots & 0 \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ & & & & K\int_R \underline{x}_k^2d\underline{x} \end{bmatrix},$$

from equation (B.6)

$$K\int_R x_i^2 d\underline{x} = \frac{1}{k+2} \, .$$

Now consider the second term of equation (B.9) and the matrix

$$K\int_R \underline{x}_2 \underline{x}_1' d\underline{x} \, .$$

That is

$$\begin{array}{c} \\ x_1^2 \\ x_2^2 \\ \cdot \\ \cdot \\ \cdot \\ x_1x_2 \\ x_1x_3 \\ \cdot \\ \cdot \\ \cdot \\ x_{k-1}x_k \end{array}
\begin{array}{c} \begin{array}{ccccc} 1 & x_1 & x_2 & \dots & x_k \end{array} \\
\left[\begin{array}{ccccc}
\frac{1}{k+2} & 0 & 0 & \dots & 0 \\
\frac{1}{k+2} & 0 & 0 & \dots & 0 \\
\cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & & \cdot \\
0 & 0 & 0 & \dots & 0 \\
0 & 0 & 0 & \dots & 0 \\
\cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & & \cdot \\
0 & 0 & 0 & \dots & 0
\end{array}\right] \end{array}$$

where the elements of the above matrix are evaluated according to equation (B.6).

Finally consider the third term of equation (B.9) and the matrix

$$K\int_R \underline{x}_2\underline{x}_2'd\underline{x} \quad ,$$

that is

$$\begin{array}{c|c}
 & \begin{array}{cccccccc} x_1^2 & x_2^2 & \cdots & x_k^2 & x_1x_2 & x_1x_3 & \cdots & x_{k-1}x_k \end{array} \\
\begin{array}{c} x_1^2 \\ x_2^2 \\ \vdots \\ x_k^2 \\ x_1x_2 \\ x_1x_3 \\ \vdots \\ x_{k-1}x_k \end{array} & \left[\begin{array}{c|c} \dfrac{2\underline{I}_k+\underline{j}_k\underline{j}_k'}{(k+2)(k+4)} & 0 \\ \hline 0 & \dfrac{\underline{I}\binom{k}{2}}{(k+2)(k+4)} \end{array}\right]
\end{array}$$

where

$$\underline{j}_k = \begin{bmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix}_{k\times 1}$$

and the main diagonal elements in the upper left hand corner are

$$K\int_R x_i^4 d\underline{x} = \frac{\Gamma\left(\frac{k+2}{2}\right)}{(\pi)^{k/2}} \cdot \frac{3/2(1/2)(\pi)^{k/2}}{\Gamma\left(\frac{k+4+1}{2}\right)}$$

$$= \frac{3}{(k+4)(k+2)}$$

The off-diagonal elements of the upper left corner and the diagonal elements of the lower right hand corner are

$$K\int_R x_i^2 x_j^2 d\underline{x} = \frac{\Gamma\left(\frac{k+1}{2}\right)}{(\pi)^{k/2}} \cdot \frac{1/4(\pi)^{k/2}}{\Gamma\left(\frac{k+4+1}{2}\right)}$$

$$= \frac{1}{(k+4)(k+2)}$$

The off-diagonal elements in the lower right hand corner are zero. Now, substituting the above matrices into equation (B.9) and performing the required algebra

$$B = \frac{1}{k+2} \sum_{g=1}^{k} \{ \sum_{i=1}^{k} \sum_{j=i}^{k} \alpha_{ij} \sum_{k=1}^{k} c^{gh} [hij] \}^2 \tag{B.10}$$

$$+\{ \sum_{i=1}^{k} \sum_{j=1}^{k} \alpha_{ij} ([ij] - \delta_{ij}/(k+2)) \}^2$$

$$\frac{+2(k+2) \sum_{i=1}^{k} \alpha_{ii}^2 + (k+2) \sum_{i=1}^{k} \sum_{j=i+1}^{k} \alpha_{ij}^2 - 2 (\sum_{i=1}^{k} \alpha_{ii})^2}{(k+2)^2 (k+4)}$$

APPENDIX C

TABLES OF DESIGN CRITERIA

The determinant of the ($\underline{X}'\underline{X}$) matrix, average squared bias, minimum mean square error, improvement ratio, and the value of the minimization function for each experimental design considered are tabulated in tables four through twenty. In addition each criterion is computed for each additional observation added to the initial experimental design, and each criterion is computed for each of three β_{ij}/σ ratios. The improvement ratio compares J for the initial undesigned experiment, say J_I, to J for the final augmented design, say J_F. Since J is a function of the number of observations N, a correction factor for J_I and J_F must be applied. The J value for a perfectly designed all-bias experiment of the same design dimensions as the undesigned experiment, say J_{ABI}, is subtracted from J_I, and in similar fashion J for a designed all-bias experiment of the same dimensions as the final augmented experiment, say J_{ABF}, is subtracted from J_F. Now the improvement ratio may be expressed as

$$IR = \frac{J_F - J_{ABF}}{J_I - J_{ABI}} .$$

The step number notation designates the number of sequentially added observations. That is, step number zero refers to the initial design, step number one refers to the initial design with one augmented observation, step number two refers to the initial design with two augmented observations, and so forth. The test case number refers to a particular replication of any given design.

The tables are arranged so that the relative contribution, of average variance and average squared bias to the minimum mean square error can be easily compared. For each of the β_{ij}/σ ratios considered in this investigation, it is easily seen that bias dominates minimum square error in every test case and design arrangement considered.

Table 3. Experimental Design Data for N=4, k=2, M=4, $\beta_{ij}/\sigma=5$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	.103	.300	.921	.637	1.495	4.474	2.073	2.362	1.624	.833
1	4.002	8.181	6.391	7.224	7.820	7.107	9.265	12.427	7.999	7.272
2	7.346	11.431	21.258	14.441	11.543	8.989	12.126	16.781	12.088	16.539
3	11.260	18.231	68.050	25.280	21.681	14.643	16.295	19.755	20.701	40.747
4	15.042	26.264	92.689	37.791	31.149	23.174	24.039	24.468	28.890	49.510
STEP NO.					AVERAGE VARIANCE					
0	39.906	23.867	5.385	5.718	4.582	2.929	4.085	4.724	4.437	5.738
1	3.807	3.076	3.647	3.601	3.196	3.183	2.864	2.611	3.095	3.599
2	3.733	3.291	2.703	3.252	3.430	3.539	3.152	2.808	3.265	3.172
3	3.854	3.201	2.226	3.029	3.061	3.445	3.320	3.099	3.075	2.498
4	4.086	3.212	2.245	2.939	3.061	3.359	3.308	3.295	3.119	2.653
STEP NO.					AVERAGE SQUARED BIAS					
0	639.114	4018.904	484.395	998.190	269.432	16.338	91.839	265.778	191.725	1037.730
1	46.148	20.278	22.703	32.492	34.106	20.771	19.512	21.857	32.935	33.216
2	22.458	24.377	80.250	32.809	27.524	24.593	22.760	22.436	25.720	66.881
3	29.471	23.447	78.097	30.498	32.500	25.063	28.224	25.741	31.293	40.413
4	28.283	27.892	72.347	29.776	29.358	30.753	27.248	30.516	29.629	36.176
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	679.019	4042.772	489.780	1003.908	274.014	19.267	95.925	270.502	196.162	1043.468
1	49.955	23.354	26.350	36.093	37.301	23.953	22.376	24.468	36.030	36.815
2	26.191	27.668	82.953	36.060	30.954	28.132	25.912	25.244	28.985	70.053
3	33.325	26.648	80.323	33.527	35.561	28.508	31.543	28.840	34.367	42.911
4	32.369	31.104	74.591	32.715	32.418	34.112	30.556	33.810	32.747	38.829
STEP NO.					IMPROVEMENT RATIO					
1	.069	.005	.047	.032	.124	1.289	.203	.078	.168	.032
2	.033	.006	.163	.032	.101	1.546	.240	.080	.131	.064
3	.044	.006	.157	.030	.117	1.562	.299	.093	.158	.038
4	.042	.007	.145	.029	.105	1.910	.287	.112	.149	.033
STEP NO.					MINIMIZATION FUNCTION					
0	1.075	2.874	5.676	7.921	4.405	1.072	2.242	3.049	3.566	8.064
1	.595	1.145	2.668	4.097	1.944	.798	.553	1.085	1.430	4.191
2	.623	.945	21.175	3.005	1.458	.926	.405	.658	1.014	7.568
3	.752	.868	53.563	1.908	.759	1.012	.511	.588	.517	2.206
4	1.116	.609	13.304	1.240	.463	.827	.454	.739	.336	1.390

Table 4. Experimental Design Data for N=5, k=2, M=5, $\beta_{ij}/\sigma=5$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.	DETERMINANT OF THE (X X) MATRIX									
0	7.577	6.023	4.381	4.957	7.647	8.367	6.738	6.037	5.776	6.809
1	15.491	17.281	10.393	21.665	15.862	14.156	12.096	17.054	13.426	10.534
2	23.410	21.293	27.369	28.497	23.823	17.884	16.523	20.137	15.934	16.926
3	30.154	25.624	42.165	34.015	30.560	22.268	24.165	28.915	24.555	23.381
4	38.969	35.890	56.849	45.011	39.506	30.220	32.399	40.205	33.552	31.242
5	49.582	50.153	72.223	64.696	50.363	41.496	45.505	49.558	43.441	43.454
STEP NO.	AVERAGE VARIANCE									
0	3.168	3.328	4.411	3.655	3.158	2.948	3.258	3.866	3.378	3.259
1	2.946	2.815	4.186	2.660	2.924	2.965	3.144	2.857	3.049	3.345
2	2.947	3.074	3.010	2.861	2.932	3.195	3.290	3.153	3.367	3.264
3	3.086	3.304	2.890	3.095	3.075	3.399	3.309	3.138	3.287	3.340
4	3.171	3.275	2.889	3.134	3.158	3.461	3.389	3.135	3.333	3.422
5	3.246	3.233	2.933	3.015	3.229	3.484	3.344	3.247	3.401	3.413
STEP NO.	AVERAGE SQUARED BIAS									
0	67.410	108.353	35.302	343.738	71.634	19.265	17.851	40.871	37.185	17.195
1	24.831	22.693	58.518	35.240	25.322	20.565	21.440	20.597	18.984	22.293
2	27.872	23.426	27.674	33.076	28.153	23.922	25.711	22.177	22.783	24.210
3	28.119	25.728	26.712	31.475	28.370	28.728	27.125	25.198	26.577	27.576
4	32.267	29.225	31.028	31.544	32.435	30.487	29.759	28.432	29.291	30.994
5	34.057	32.612	32.463	33.603	34.060	33.697	34.808	31.888	33.547	32.291
STEP NO.	MINIMUM MEAN SQUARE ERROR									
0	70.578	111.681	39.713	347.393	74.792	22.212	21.109	44.738	40.563	20.455
1	27.777	25.508	62.703	37.900	28.247	23.530	24.584	23.454	22.034	25.638
2	30.819	26.500	30.684	35.936	31.085	27.117	29.001	25.329	26.150	27.474
3	31.205	29.032	29.602	34.571	31.445	32.127	30.434	28.337	29.863	30.916
4	35.438	32.500	33.918	34.678	35.593	33.948	33.148	31.567	32.623	34.416
5	37.303	35.846	35.396	36.618	37.290	37.181	38.153	35.135	36.947	35.704
STEP NO.	IMPROVEMENT RATIO									
1	.359	.201	1.634	.099	.344	1.064	1.192	.479	.495	1.301
2	.402	.209	.743	.093	.382	1.250	1.437	.522	.603	1.402
3	.406	.232	.709	.089	.386	1.513	1.512	.592	.700	1.599
4	.468	.263	.825	.089	.442	1.605	1.660	.667	.772	1.800
5	.494	.292	.863	.094	.464	1.772	1.939	.751	.885	1.869
STEP NO.	MINIMIZATION FUNCTION									
0	2.235	2.965	8.385	7.122	2.378	.693	1.013	2.231	1.719	.854
1	1.109	.699	6.017	2.940	1.169	.207	.655	.794	.584	.772
2	.579	.425	4.501	1.994	.622	.209	.656	.642	.671	.559
3	.431	.469	3.361	1.498	.456	.403	.774	.519	.637	.702
4	.353	.440	2.684	1.248	.363	.594	.749	.209	.487	.768
5	.437	.347	2.083	.694	.425	.713	.704	.358	.756	.911

Table 5. Experimental Design Data for N=8, k=2, M=5, $\beta_{ij}/\sigma=5$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	27.022	39.586	46.243	36.379	31.249	35.084	31.430	12.733	25.370	18.940
1	57.789	71.742	64.288	55.664	44.051	60.830	44.482	42.761	51.218	32.373
2	47.722	82.065	73.181	81.122	53.113	70.829	54.544	60.383	63.886	46.472
3	65.074	91.551	80.508	103.477	68.720	78.271	72.203	84.966	83.126	60.721
4	89.849	105.896	97.543	114.614	90.101	90.850	89.793	110.558	104.894	85.416
5	115.374	134.837	121.886	124.447	107.937	108.774	107.007	133.863	125.737	104.981
STEP NO.					AVERAGE VARIANCE					
0	3.180	2.861	2.743	2.886	3.035	2.951	3.029	4.314	3.262	3.725
1	3.199	2.631	2.722	2.853	3.067	2.736	3.069	3.153	2.921	3.397
2	3.290	2.791	2.886	2.784	3.191	2.883	3.169	3.130	3.029	3.352
3	3.270	2.958	3.074	2.805	3.205	3.067	3.152	3.032	3.027	3.359
4	3.195	3.063	3.129	2.951	3.191	3.182	3.193	3.002	3.040	3.249
5	3.184	3.035	3.130	3.113	3.263	3.247	3.268	3.039	3.093	3.292
STEP NO.					AVERAGE SQUARED BIAS					
0	37.568	45.553	39.488	28.391	31.777	46.593	35.429	209.798	53.808	32.628
1	45.614	36.447	36.431	34.195	32.385	42.671	33.899	31.965	30.277	33.815
2	51.889	35.923	36.199	36.991	36.179	45.019	36.729	33.781	32.067	33.196
3	58.983	36.949	37.581	39.334	41.568	49.421	42.509	41.590	34.933	37.913
4	41.495	38.793	39.340	40.885	39.642	50.190	42.970	42.728	37.598	39.105
5	46.828	43.578	43.010	43.608	43.852	55.555	48.174	47.335	40.710	42.299
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	40.748	48.414	42.232	31.277	34.813	49.544	38.459	214.112	57.070	36.353
1	48.813	39.078	39.153	37.048	35.452	45.407	36.968	35.118	33.198	37.212
2	55.179	38.714	39.085	39.775	39.370	47.902	39.898	36.911	35.096	36.548
3	62.253	39.908	40.655	42.140	44.773	52.487	45.662	44.622	37.960	41.272
4	44.690	41.857	42.469	43.836	42.833	53.373	46.164	45.730	40.639	42.354
5	50.013	46.613	46.140	46.722	47.116	58.803	51.441	50.374	43.803	45.591
STEP NO.					IMPROVEMENT RATIO					
1	1.216	.787	.916	1.207	1.017	.906	.953	.148	.548	1.023
2	1.386	.776	.911	1.302	1.140	.958	1.035	.155	.581	.998
3	1.575	.800	.949	1.385	1.311	1.056	1.198	.192	.633	1.140
4	1.094	.841	.993	1.442	1.244	1.073	1.209	.196	.681	1.170
5	1.235	.945	1.086	1.543	1.379	1.190	1.359	.218	.738	1.266
STEP NO.					MINIMIZATION FUNCTION					
0	1.777	5.439	1.886	4.747	1.026	3.277	1.316	8.741	4.789	1.708
1	1.647	2.623	1.069	3.389	.589	1.487	.750	3.499	1.598	1.112
2	1.851	1.910	.655	2.216	.607	1.129	.750	2.411	1.013	.982
3	1.697	1.509	.520	1.549	.595	1.074	.540	1.474	.591	1.006
4	1.165	1.351	.577	1.292	.545	1.233	.535	.998	.258	.632
5	.941	.928	.343	1.304	.609	1.272	.679	.653	.153	.675

Table 6. Experimental Design Data for N=6, k=3, M=4, $\beta_{ij}/\sigma=5$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.	DETERMINANT OF THE (X X) MATRIX									
0	.443	.421	.513	1.545	.052	.365	.097	.038	.069	1.733
1	11.219	3.222	3.893	7.329	.816	3.459	.710	.159	.892	31.729
2	18.277	11.710	25.545	10.305	5.808	6.445	13.795	6.510	4.570	47.699
3	32.799	26.059	50.664	22.492	19.594	10.961	35.258	15.174	19.138	67.147
4	47.531	40.358	70.278	48.012	40.544	29.757	51.715	31.387	42.586	92.170
STEP NO.	AVERAGE VARIANCE									
0	24.650	11.930	30.874	7.970	35.215	15.364	83.305	69.482	32.629	11.195
1	4.991	8.967	11.949	6.743	18.811	7.008	37.879	74.144	17.533	3.690
2	4.909	5.670	4.612	7.374	8.271	6.964	5.590	7.227	10.051	3.854
3	4.575	4.968	4.114	6.061	5.747	7.161	4.567	6.549	5.975	3.985
4	4.614	4.858	4.177	4.962	4.961	5.272	4.617	5.529	4.930	4.062
STEP NO.	AVERAGE SQUARED BIAS									
0	3107.035	458.282	88.729	145.680	448.351	192.755	412.109	159.181	344.976	7662.497
1	57.649	71.651	491.496	33.740	61.389	54.232	1948.242	919.179	85.833	54.279
2	66.492	65.818	50.335	40.493	108.494	54.678	58.984	65.332	138.664	48.409
3	76.532	76.941	66.382	51.025	74.959	37.889	60.539	~~53.118~~	~~92.888~~	49.718
4	83.935	52.249	64.992	56.396	50.181	46.840	63.827	51.061	52.909	48.451
STEP NO.	MINIMUM MEAN SQUARE ERROR									
0	3131.686	470.212	119.603	153.649	483.566	208.119	495.414	228.662	377.605	7673.692
1	62.640	80.618	503.445	40.483	80.200	61.241	1986.122	993.323	103.365	57.968
2	71.401	71.488	54.947	47.867	116.765	61.642	64.575	72.559	148.715	52.264
3	81.107	81.909	70.496	57.086	80.706	45.050	65.106	59.667	98.863	53.703
4	88.549	57.108	69.169	61.358	55.142	52.113	68.444	56.590	57.839	52.513
STEP NO.	IMPROVEMENT RATIO									
1	.018	.162	4.346	.238	.157	.276	4.039	4.417	.264	.007
2	.021	.142	.434	.287	.233	.278	.121	.301	.385	.006
3	.024	.164	.568	.348	.157	.195	.122	.243	.251	.006
4	.027	.111	.555	.375	.104	.229	.128	.228	.148	.006
STEP NO.	MINIMIZATION FUNCTION									
0	3.718	5.242	6.330	9.069	5.028	2.601	5.330	5.810	5.327	13.010
1	1.995	2.801	4.806	4.555	3.508	1.808	3.464	3.050	3.675	7.705
2	1.980	2.665	3.795	3.886	3.231	2.262	2.966	2.643	3.487	6.087
3	1.746	1.870	3.052	3.318	2.702	2.212	1.939	1.845	2.883	5.100
4	1.827	1.830	2.802	2.717	2.211	2.100	1.782	2.011	2.335	4.158

Table 7. Experimental Design Data for N=8, k=3, M=5, $\beta_{ij}/\sigma=5$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.	DETERMINANT OF THE (X X) MATRIX									
0	4.474	9.431	8.936	18.169	18.885	7.605	17.021	4.977	2.895	1.330
1	23.216	44.205	29.414	68.077	76.735	41.551	74.273	19.358	13.493	7.336
2	53.396	72.325	60.655	95.766	110.619	56.518	108.068	47.368	42.532	18.942
3	86.731	108.938	148.778	130.807	146.641	98.237	144.568	82.418	77.777	36.273
4	112.530	138.968	178.627	163.192	180.646	148.830	178.215	105.846	102.414	74.217
5	146.552	180.490	232.431	192.312	208.199	186.144	204.458	138.055	158.148	100.150
STEP NO.	AVERAGE VARIANCE									
0	8.644	6.638	6.421	5.180	5.226	7.364	5.376	7.797	9.010	13.458
1	5.555	4.434	5.570	3.851	3.762	4.647	3.800	5.992	7.507	7.229
2	4.578	4.286	4.740	3.899	3.776	4.761	3.813	4.692	5.236	6.358
3	4.369	4.174	3.844	3.936	3.848	4.287	3.881	4.398	4.822	5.557
4	4.468	4.264	4.003	4.038	3.957	4.127	3.994	4.517	4.922	4.964
5	4.497	4.314	4.047	4.192	4.127	4.217	4.173	4.557	4.636	5.028
STEP NO.	AVERAGE SQUARED BIAS									
0	195.940	170.026	172.370	171.950	270.171	672.587	359.128	334.377	181.312	65.167
1	60.585	53.863	82.972	42.837	51.206	45.323	47.330	129.490	69.373	80.353
2	51.457	44.058	132.651	45.177	52.466	43.195	47.649	117.106	46.703	70.543
3	44.715	49.994	55.435	45.332	52.084	48.442	47.754	56.205	52.907	100.652
4	51.686	50.967	60.402	49.268	55.210	47.726	50.115	63.633	60.201	60.142
5	55.627	58.534	57.299	52.690	58.691	52.247	53.475	70.781	58.546	53.317
STEP NO.	MINIMUM MEAN SQUARE ERROR									
0	204.584	176.664	178.792	177.130	275.397	679.951	364.504	342.175	190.322	78.625
1	66.140	58.297	88.542	46.688	54.968	49.970	51.130	135.481	76.880	87.582
2	56.035	48.344	137.391	49.075	56.242	47.955	51.463	121.798	51.939	76.901
3	49.084	54.169	59.279	49.268	55.931	52.729	51.635	60.603	57.729	106.209
4	56.154	55.230	64.405	53.307	59.167	51.853	54.109	68.150	65.123	65.106
5	60.123	62.847	61.345	56.882	62.819	56.463	57.648	75.338	63.182	58.345
STEP NO.	IMPROVEMENT RATIO									
1	.305	.309	.479	.240	.184	.066	.127	.386	.386	1.120
2	.253	.250	.760	.253	.188	.063	.128	.345	.251	.972
3	.218	.283	.309	.253	.186	.070	.128	.163	.281	1.370
4	.252	.288	.337	.276	.197	.068	.134	.185	.320	.807
5	.271	.332	.319	.296	.210	.075	.144	.206	.309	.713
STEP NO.	MINIMIZATION FUNCTION									
0	6.794	8.889	11.821	6.544	8.158	6.709	9.003	5.233	12.481	3.314
1	4.238	4.989	7.778	2.946	4.039	3.438	4.425	2.971	7.149	3.484
2	3.272	3.925	9.477	2.173	3.031	3.200	3.359	2.588	5.717	2.584
3	2.547	3.095	5.137	1.676	2.378	2.776	2.608	1.649	4.271	3.038
4	2.588	2.973	4.627	1.369	1.979	2.252	2.196	1.782	4.020	2.022
5	2.783	2.806	3.804	1.373	1.909	2.192	2.105	1.976	3.889	2.253

Table 8. Experimental Design Data for N=10, k=3, M=7, $\beta_{ij}/\sigma=5$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	8.824	11.062	.763	3.774	6.781	10.872	22.997	6.679	8.310	11.477
1	51.881	26.698	5.269	29.125	30.230	40.452	67.822	35.469	21.731	41.284
2	96.822	64.468	105.697	55.894	72.972	68.285	108.594	81.165	49.425	101.864
3	193.797	128.734	258.152	128.492	127.495	115.479	148.890	129.344	95.696	168.851
4	257.430	304.540	548.603	160.583	162.672	213.017	223.950	160.865	214.875	212.635
5	301.352	378.132	960.229	224.903	227.699	322.513	331.962	241.533	288.331	303.129
6	408.142	544.506	1248.320	9014.792	297.236	403.556	391.225	313.702	379.297	366.848
7	545.334	695.342	1444.868	40393.281	478.625	518.174	478.559	455.287	479.775	439.149
STEP NO.					AVERAGE VARIANCE					
0	11.692	8.291	30.829	12.786	9.131	7.275	6.742	11.429	7.801	8.872
1	6.022	7.438	21.577	6.632	6.370	5.662	4.838	6.047	7.224	5.977
2	5.005	5.599	6.223	5.597	5.000	5.580	4.648	4.915	6.586	4.627
3	4.253	4.756	5.571	4.638	4.663	5.148	4.649	4.707	5.407	4.358
4	4.226	4.170	4.240	4.743	4.759	4.486	4.391	4.816	4.423	4.425
5	4.362	4.225	3.680	4.690	4.685	4.263	4.223	4.599	4.398	4.312
6	4.277	4.013	3.603	3.501	4.668	4.304	4.322	4.611	4.363	4.394
7	4.218	3.981	3.667	2.625	4.358	4.276	4.360	4.413	4.352	4.458
STEP NO.					AVERAGE SQUARED BIAS					
0	782.950	117.795	1452.431	644.832	248.011	332.390	116.992	125.269	97.401	142.261
1	54.982	116.612	159.018	113.840	97.821	103.452	47.766	164.723	93.505	137.514
2	65.586	104.239	782.680	116.346	85.675	98.627	55.273	78.764	66.902	66.843
3	67.437	141.653	250.280	104.935	97.055	63.082	58.276	88.994	58.758	82.775
4	72.672	61.401	201.903	107.386	106.994	83.219	59.653	98.113	65.253	91.179
5	79.467	62.733	142.155	112.013	116.170	63.994	64.535	113.611	78.758	75.635
6	85.668	67.278	136.068	23046.294	123.146	68.207	68.504	117.838	68.422	82.983
7	73.787	70.376	135.702	26479.685	68.533	74.219	74.841	71.817	75.246	91.354
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	794.642	126.087	1483.260	657.618	257.142	339.665	123.733	136.698	105.202	151.133
1	61.004	124.049	180.595	120.471	104.191	109.114	52.604	170.769	100.729	143.491
2	70.591	109.838	788.903	121.943	90.676	104.207	59.921	83.678	73.488	71.470
3	71.690	146.409	255.852	109.574	101.718	68.230	62.925	93.701	65.165	87.133
4	76.898	65.571	206.142	112.129	111.753	87.705	64.044	102.929	69.676	95.605
5	83.829	66.958	145.835	116.704	120.855	68.257	68.754	118.210	75.148	79.948
6	89.945	71.291	139.671	23049.795	127.814	72.510	72.826	122.449	72.785	87.377
7	78.005	74.357	139.370	26482.310	72.891	78.495	79.201	76.230	79.598	95.812
STEP NO.					IMPROVEMENT RATIO					
1	.070	.982	.118	.176	.391	.310	.397	1.259	.954	.946
2	.082	.863	.530	.178	.337	.294	.457	.593	.679	.451
3	.083	1.165	.169	.159	.380	.186	.482	.669	.594	.557
4	.090	.493	.135	.163	.420	.244	.490	.738	.637	.614
5	.098	.503	.094	.169	.455	.185	.528	.853	.691	.506
6	.106	.538	.090	35.338	.482	.198	.561	.884	.665	.556
7	.090	.562	.090	40.602	.263	.215	.614	.531	.732	.613
STEP NO.					MINIMIZATION FUNCTION					
0	9.306	6.832	12.902	9.136	7.598	11.704	4.444	6.672	8.472	5.595
1	5.249	4.553	7.905	5.838	5.068	6.788	3.406	4.403	5.284	3.671
2	4.620	4.521	479.244	5.[illegible]76	4.529	5.039	2.745	4.191	4.337	3.369
3	3.950	15.215	65.196	4.523	3.568	3.987	2.324	3.119	4.179	2.293
4	3.410	11.036	60.802	4.765	3.653	3.496	2.145	3.260	2.528	2.209
5	3.386	3.732	57.309	4.[illegible]23	3.332	2.158	1.228	2.877	2.182	1.811
6	3.016	2.607	53.834	************	3.362	2.083	1.391	2.913	1.964	1.534
7	2.216	2.067	51.406	646204.575	1.348	1.850	1.502	1.979	2.211	2.150

Table 9. Experimental Design Data for N=4, k=2, M=4, $\beta_{ij}/\sigma=10$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	.103	.300	.021	.837	1.495	4.474	2.073	2.362	1.624	.833
1	4.092	3.181	6.391	7.224	7.620	7.107	9.265	12.427	7.999	7.272
2	7.346	11.431	21.256	14.441	11.543	8.989	12.126	16.781	12.088	16.539
3	11.260	18.231	68.050	25.280	21.081	14.643	16.293	19.755	20.701	40.747
4	15.042	26.264	92.689	37.791	31.149	23.174	24.039	24.468	28.890	49.510
STEP NO.					AVERAGE VARIANCE					
0	39.906	23.867	5.385	5.718	4.582	2.929	4.065	4.724	4.437	5.738
1	3.807	3.076	3.647	3.601	3.196	3.183	2.864	2.611	3.095	3.599
2	3.733	3.291	2.705	3.252	3.430	3.539	3.152	2.808	3.265	3.172
3	3.854	3.201	2.226	3.029	3.061	3.445	3.326	3.099	3.075	2.498
4	4.086	3.212	2.245	2.939	3.061	3.359	3.306	3.295	3.119	2.653
STEP NO.					AVERAGE SQUARED BIAS					
0	2556.454	16075.617	1937.579	3992.760	1077.730	65.353	367.357	1063.112	766.901	4150.918
1	184.593	61.110	90.811	129.969	136.423	83.083	78.047	87.427	131.738	132.863
2	89.831	97.509	321.006	131.234	110.096	98.371	91.039	89.744	102.880	267.524
3	117.884	93.788	312.387	121.991	129.999	100.252	112.894	102.964	125.170	161.651
4	113.132	111.567	289.387	119.103	117.431	123.011	108.991	122.062	118.514	144.703
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	2596.360	16099.484	1942.964	3998.479	1082.311	68.282	371.442	1067.836	771.338	4156.656
1	186.399	64.186	94.456	133.570	139.618	86.265	80.911	90.038	134.833	136.462
2	93.564	100.799	323.705	134.486	113.526	101.910	94.191	92.552	106.144	270.696
3	121.738	96.989	314.613	125.020	133.060	103.697	116.214	106.063	128.245	164.150
4	117.216	114.779	291.631	122.043	120.492	126.371	112.299	125.357	121.633	147.357
STEP NO.					IMPROVEMENT RATIO					
1	.071	.005	.047	.033	.126	1.276	.216	.081	.171	.032
2	.035	.006	.165	.033	.102	1.515	.246	.083	.133	.064
3	.085	.006	.160	.030	.120	1.541	.305	.096	.162	.039
4	.084	.007	.148	.030	.108	1.889	.294	.114	.153	.035
STEP NO.					MINIMIZATION FUNCTION					
0	1.175	2.874	5.676	7.921	4.405	1.072	2.242	3.049	3.566	8.064
1	.595	1.145	2.666	4.097	1.944	.798	.553	1.085	1.430	4.191
2	.623	.945	21.175	3.005	1.458	.926	.403	.658	1.014	7.568
3	.752	.668	53.563	1.908	.759	1.012	.511	.588	.517	2.206
4	1.116	.609	13.304	1.240	.463	.827	.454	.739	.336	1.390

Table 10. Experimental Design Data for N=5, k=2, M=5, $\beta_{ij}/\sigma=10$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X'X) MATRIX					
0	7.577	6.023	4.781	4.957	7.647	8.367	6.730	6.037	5.776	6.809
1	15.491	17.281	10.395	21.665	15.862	14.156	12.096	17.054	13.426	10.534
2	25.410	21.293	27.369	28.497	25.825	17.884	16.525	20.137	15.934	16.926
3	30.154	25.624	42.165	34.015	30.560	22.268	24.165	28.915	24.555	23.381
4	36.969	35.890	56.849	45.011	39.506	30.220	32.399	40.265	33.552	31.242
5	49.582	50.153	72.225	64.696	50.363	41.496	45.505	49.558	43.441	43.454

STEP NO.					AVERAGE VARIANCE					
0	3.166	3.328	4.411	3.655	3.158	2.948	3.250	3.606	3.376	3.259
1	2.946	2.815	4.186	2.660	2.924	2.965	3.144	2.857	3.049	3.345
2	2.947	3.074	3.010	2.861	2.932	3.195	3.290	3.153	3.367	3.264
3	3.096	3.304	2.890	3.095	3.075	3.399	3.309	3.138	3.287	3.340
4	3.171	3.275	2.889	3.134	3.158	3.461	3.389	3.135	3.335	3.422
5	3.286	3.233	2.935	3.015	3.229	3.484	3.344	3.247	3.401	3.413

STEP NO.					AVERAGE SQUARED BIAS					
0	269.641	433.411	141.206	1374.951	286.536	77.059	71.402	163.466	148.740	68.782
1	99.325	90.772	234.071	140.959	101.289	82.259	85.761	82.387	75.938	89.171
2	111.486	93.704	110.695	132.303	112.613	95.688	102.640	88.706	91.132	96.840
3	112.478	102.911	106.846	125.902	113.480	114.912	108.496	100.794	106.307	110.304
4	129.067	116.698	124.114	126.177	129.741	121.949	119.037	113.727	117.162	123.975
5	136.279	130.450	129.855	134.410	136.242	134.789	139.235	127.553	134.187	129.166

STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	272.896	436.740	145.619	1378.605	289.694	80.006	74.660	167.352	152.117	72.041
1	102.271	93.588	238.257	143.619	104.214	85.224	88.905	85.244	78.987	92.516
2	114.435	96.778	113.705	135.163	115.545	98.883	106.135	91.859	94.499	100.104
3	115.563	106.215	109.736	128.997	116.556	118.311	111.606	103.932	109.593	113.644
4	132.236	120.174	127.005	129.311	132.899	125.410	122.426	116.862	120.495	127.397
5	139.475	133.683	132.786	137.426	139.471	138.272	142.577	130.800	137.586	132.578

STEP NO.					IMPROVEMENT RATIO					
1	.366	.207	1.652	.102	.351	1.067	1.199	.498	.507	1.297
2	.411	.214	.773	.095	.390	1.244	1.440	.537	.610	1.407
3	.414	.236	.745	.091	.393	1.497	1.516	.610	.711	1.603
4	.476	.268	.865	.091	.450	1.586	1.665	.669	.784	1.802
5	.502	.299	.905	.097	.473	1.755	1.947	.773	.898	1.876

STEP NO.					MINIMIZATION FUNCTION					
0	2.235	2.965	8.385	7.122	2.378	.693	1.015	2.231	1.719	.854
1	1.199	.699	6.017	2.940	1.169	.207	.655	.794	.584	.772
2	.579	.425	4.501	1.994	.622	.209	.650	.642	.671	.559
3	.431	.459	3.361	1.498	.456	.403	.774	.519	.637	.702
4	.355	.440	2.684	1.248	.363	.594	.749	.200	.487	.768
5	.437	.347	2.685	.694	.425	.713	.704	.358	.756	.911

Table 11. Experimental Design Data for N=8, k=2, M=5, $\beta_{ij}/\sigma=10$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	21.972	39.586	46.243	36.379	31.249	35.084	31.430	12.733	25.370	18.940
1	37.799	71.742	64.286	55.664	44.051	60.830	44.482	42.761	51.216	32.373
2	47.772	82.065	73.181	81.122	53.113	70.829	54.544	60.383	63.886	46.472
3	65.074	91.551	80.506	103.477	68.720	78.271	72.203	84.966	83.126	60.721
4	89.849	105.696	97.543	114.814	90.101	90.850	89.793	110.558	104.894	85.416
5	115.374	134.837	121.886	124.447	107.937	108.774	107.007	133.863	125.737	104.981
STEP NO.					AVERAGE VARIANCE					
0	3.190	2.861	2.743	2.886	3.035	2.951	3.029	4.314	3.262	3.725
1	3.199	2.631	2.722	2.853	3.067	2.736	3.069	3.153	2.921	3.397
2	3.290	2.791	2.886	2.784	3.191	2.883	3.169	3.130	3.029	3.352
3	3.274	2.958	3.074	2.805	3.205	3.067	3.152	3.032	3.027	3.359
4	3.195	3.063	3.129	2.951	3.191	3.182	3.193	3.002	3.040	3.249
5	3.184	3.035	3.130	3.113	3.263	3.247	3.260	3.039	3.093	3.292
STEP NO.					AVERAGE SQUARED BIAS					
0	150.270	162.212	157.954	113.563	127.110	186.372	141.717	839.192	215.231	130.512
1	182.455	145.790	145.726	136.779	129.541	170.684	135.593	127.859	121.109	135.260
2	207.557	143.692	144.798	147.964	144.715	180.076	146.913	135.124	128.268	132.784
3	235.930	147.797	150.324	157.338	166.271	197.682	170.036	166.361	139.731	151.651
4	165.979	155.174	157.359	163.540	158.569	200.761	171.661	170.911	150.393	156.419
5	187.313	174.311	172.041	174.434	175.410	222.221	192.693	189.339	162.840	169.196
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	153.450	165.073	160.697	116.449	130.145	189.323	144.746	843.507	218.494	134.238
1	185.655	148.420	148.446	139.632	132.608	173.421	138.664	131.012	124.029	138.657
2	210.847	146.483	147.684	150.748	147.907	182.959	150.084	138.254	131.297	136.136
3	239.290	150.756	153.396	160.143	169.477	200.749	173.190	169.392	142.758	155.010
4	169.174	153.237	160.486	166.491	161.760	203.944	175.073	173.914	153.434	159.668
5	190.497	177.346	175.170	177.547	178.673	225.468	195.962	192.378	165.933	172.488
STEP NO.					IMPROVEMENT RATIO					
1	1.215	.797	.921	1.205	1.019	.914	.956	.151	.559	1.033
2	1.382	.735	.913	1.303	1.139	.964	1.036	.160	.592	1.013
3	1.571	.808	.951	1.385	1.309	1.060	1.199	.197	.645	1.157
4	1.102	.849	.995	1.441	1.247	1.076	1.212	.202	.694	1.191
5	1.244	.954	1.086	1.538	1.380	1.192	1.359	.224	.752	1.289
STEP NO.					MINIMIZATION FUNCTION					
0	1.777	5.439	1.986	4.747	1.026	3.277	1.316	8.741	4.789	1.708
1	1.687	2.623	1.069	3.389	.589	1.487	.756	3.499	1.598	1.112
2	1.351	1.910	.653	2.216	.607	1.129	.750	2.411	1.013	.982
3	1.097	1.509	.520	1.549	.595	1.074	.540	1.474	.591	1.006
4	1.165	1.351	.577	1.292	.545	1.233	.533	.998	.258	.632
5	.341	.328	.343	1.304	.609	1.272	.679	.653	.153	.675

Table 12. Experimental Design Data for N=6, k=3, M=4, $\beta_{ij}/\alpha=10$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	.403	.421	.513	1.545	.052	.365	.097	.038	.069	1.733
1	11.219	3.222	3.893	7.329	.816	3.459	.710	.159	.892	31.729
2	16.277	11.710	25.843	10.305	5.608	6.445	13.795	6.510	4.570	47.699
3	32.799	26.059	50.664	22.492	19.594	10.961	35.258	15.174	19.138	67.147
4	47.531	40.356	70.276	48.012	40.544	29.757	51.715	31.387	42.586	92.170
STEP NO.					AVERAGE VARIANCE					
0	24.650	11.930	30.874	7.970	35.215	15.364	83.303	69.482	32.629	11.195
1	4.991	8.967	11.949	6.743	16.811	7.008	37.879	74.144	17.533	3.698
2	4.909	5.670	4.612	7.374	6.271	6.964	5.590	7.227	10.051	3.854
3	4.575	4.968	4.114	6.061	5.747	7.161	4.367	6.549	5.975	3.985
4	4.614	4.658	4.177	4.962	4.961	5.272	4.617	5.529	4.930	4.062
STEP NO.					AVERAGE SQUARED BIAS					
0	12426.141	1633.127	354.916	582.719	1793.404	771.021	1648.436	636.722	1379.905	30649.989
1	230.597	266.636	1965.986	134.959	245.558	216.930	7792.969	3676.717	343.330	217.115
2	265.967	263.273	201.339	161.971	433.976	218.710	235.936	261.330	554.654	193.637
3	306.126	307.765	265.526	204.102	299.635	151.556	242.157	212.472	371.550	198.874
4	335.741	208.998	259.967	225.586	200.723	187.362	255.306	204.242	211.636	193.806
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	12452.791	1645.057	385.790	590.689	1828.619	786.385	1731.743	706.204	1412.534	30661.183
1	235.587	295.572	1977.935	141.702	264.369	223.938	7830.849	3750.861	360.863	220.805
2	270.876	268.943	205.951	169.345	442.248	225.674	241.526	268.557	564.706	197.492
3	310.793	312.733	269.642	210.162	304.582	158.717	246.723	219.021	377.526	202.858
4	340.355	213.856	264.144	230.548	205.685	192.634	259.924	209.771	216.565	197.868
STEP NO.					IMPROVEMENT RATIO					
1	.019	.158	5.180	.233	.142	.280	4.532	5.341	.253	.007
2	.021	.143	.527	.280	.240	.282	.137	.375	.397	.006
3	.025	.167	.694	.350	.165	.196	.140	.305	.264	.006
4	.027	.113	.679	.384	.110	.239	.147	.291	.150	.006
STEP NO.					MINIMIZATION FUNCTION					
0	3.716	5.242	6.336	9.069	5.028	2.601	5.536	5.810	5.327	13.010
1	1.995	2.891	4.806	4.555	3.508	1.808	3.464	3.050	3.675	7.705
2	1.990	2.665	3.795	3.886	3.231	2.262	2.966	2.643	3.487	6.087
3	1.746	1.870	3.052	3.318	2.702	2.212	1.936	1.845	2.883	5.100
4	1.377	1.830	2.902	2.717	2.211	2.100	1.782	2.011	2.335	4.158

Table 13. Experimental Design Data for N=8, k=3, M=5, $\beta_{ij}/\sigma=10$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	4.474	9.431	8.936	18.169	18.885	7.005	17.021	4.977	2.895	1.330
1	23.216	44.205	29.414	68.077	76.735	41.551	74.273	19.358	13.493	7.336
2	53.396	72.325	60.655	95.766	110.619	56.518	108.060	47.368	42.532	18.942
3	86.731	108.938	148.776	130.807	146.641	98.237	144.560	82.418	77.777	36.273
4	112.530	138.968	178.627	163.192	180.646	148.830	178.215	105.846	102.414	74.217
5	146.552	180.490	232.431	192.312	208.199	186.144	204.456	138.055	158.148	100.150
STEP NO.					AVERAGE VARIANCE					
0	6.644	6.638	6.421	5.180	5.226	7.364	5.376	7.797	9.010	13.458
1	5.555	4.434	5.570	3.851	3.762	4.647	3.600	5.992	7.507	7.229
2	4.378	4.286	4.740	3.899	3.776	4.761	3.613	4.692	5.236	6.358
3	4.369	4.174	3.844	3.936	3.648	4.287	3.681	4.398	4.822	5.557
4	4.468	4.264	4.003	4.038	3.957	4.127	3.994	4.517	4.922	4.964
5	4.497	4.314	4.047	4.192	4.127	4.217	4.173	4.557	4.636	5.028
STEP NO.					AVERAGE SQUARED BIAS					
0	783.761	680.104	689.481	687.800	1080.684	2690.349	1436.511	1337.509	725.247	260.667
1	242.341	215.452	331.886	171.347	204.624	181.293	189.310	517.958	277.491	321.411
2	205.830	176.232	530.603	180.707	209.865	172.779	190.590	468.425	186.814	282.173
3	178.858	199.978	221.741	181.328	208.335	193.768	191.010	224.820	211.628	402.606
4	206.794	203.866	241.606	197.072	220.838	190.902	200.459	254.532	240.803	240.568
5	222.506	234.134	229.194	210.761	234.764	208.986	213.090	283.125	234.185	213.267
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	792.405	686.742	695.903	692.979	1085.910	2697.713	1441.880	1345.306	734.257	274.125
1	247.896	219.886	337.457	175.198	208.586	185.940	193.119	523.950	284.998	328.640
2	210.408	180.518	535.344	184.605	213.641	177.540	194.411	473.117	192.050	288.531
3	183.228	204.152	225.585	185.264	212.183	198.055	194.690	229.218	216.450	408.164
4	211.212	208.130	245.611	201.111	224.795	195.029	204.453	259.049	245.725	245.532
5	227.003	238.448	233.241	214.953	238.892	213.203	218.071	287.681	238.821	218.295
STEP NO.					IMPROVEMENT RATIO					
1	.308	.315	.481	.247	.188	.067	.131	.387	.384	1.202
2	.260	.257	.767	.260	.193	.064	.131	.349	.256	1.052
3	.226	.291	.318	.261	.191	.071	.132	.167	.289	1.497
4	.261	.297	.347	.284	.203	.070	.136	.169	.329	.891
5	.281	.341	.329	.304	.216	.077	.140	.210	.319	.790
STEP NO.					MINIMIZATION FUNCTION					
0	6.794	8.889	11.821	6.544	8.158	6.709	9.003	5.233	12.481	3.314
1	4.238	4.989	7.776	2.946	4.039	3.438	4.423	2.971	7.149	3.484
2	3.272	3.925	9.477	2.173	3.031	3.200	3.359	2.508	5.717	2.584
3	2.547	3.095	5.137	1.676	2.378	2.776	2.600	1.649	4.271	3.038
4	2.586	2.973	4.627	1.369	1.979	2.252	2.190	1.762	4.020	2.022
5	2.793	2.806	3.804	1.373	1.909	2.192	2.103	1.976	3.889	2.253

Table 14. Experimental Design Data for N=10, k=3, M=7, β_{ij}/σ=10

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X'X) MATRIX					
0	6.824	11.062	.765	3.774	6.781	10.872	22.997	6.679	8.310	11.477
1	51.391	26.698	5.269	29.125	30.230	40.452	67.026	35.469	21.731	41.284
2	96.892	64.468	105.697	55.894	72.972	68.285	108.594	81.165	49.425	101.864
3	195.797	128.734	258.152	128.492	127.495	115.479	148.690	126.344	95.696	168.851
4	257.430	304.540	540.683	160.583	162.672	213.017	223.950	160.865	214.875	212.635
5	301.352	378.132	960.929	224.903	227.699	322.513	331.962	241.533	288.331	303.129
6	406.142	544.506	1248.920	9014.792	297.236	403.556	391.225	313.702	379.297	366.848
7	545.334	695.392	1444.966	40393.281	476.025	518.174	478.559	455.267	479.775	439.149
STEP NO.					AVERAGE VARIANCE					
0	11.692	8.291	30.929	12.786	9.131	7.275	6.742	11.429	7.801	8.872
1	6.092	7.438	21.677	6.632	6.370	5.662	4.630	6.047	7.224	5.977
2	5.005	5.599	6.225	5.597	5.000	5.580	4.646	4.915	6.586	4.627
3	4.253	4.756	5.571	4.638	4.663	5.148	4.649	4.707	5.407	4.358
4	4.296	4.170	4.240	4.743	4.759	4.486	4.391	4.816	4.425	4.425
5	4.362	4.225	3.686	4.690	4.685	4.263	4.223	4.599	4.390	4.312
6	4.277	4.013	3.603	3.591	4.668	4.304	4.322	4.611	4.363	4.394
7	4.218	3.981	3.667	2.625	4.358	4.276	4.360	4.413	4.352	4.458
STEP NO.					AVERAGE SQUARED BIAS					
0	3131.892	471.181	5809.723	2579.330	992.044	1329.560	467.966	501.077	369.602	569.043
1	219.926	466.496	636.073	455.359	391.284	413.808	191.066	658.891	374.019	550.055
2	262.385	416.956	5130.722	465.385	342.701	394.507	221.092	315.054	267.608	267.372
3	269.749	566.011	1001.122	419.742	388.221	252.328	233.102	355.977	239.032	331.182
4	290.689	245.605	807.610	429.546	427.977	332.875	238.614	392.453	261.013	364.717
5	317.367	250.934	568.620	448.054	464.682	255.974	258.142	454.444	283.031	382.542
6	342.672	269.112	544.275	92185.177	492.584	272.826	274.015	471.352	273.688	331.931
7	295.149	261.506	542.809	105918.741	274.130	296.876	299.360	287.269	300.985	365.417
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	3143.494	479.472	5840.652	2592.116	1001.175	1336.836	474.706	512.506	397.403	577.915
1	225.950	473.684	657.650	461.990	397.654	419.471	195.903	664.937	381.243	556.032
2	267.389	422.555	5136.945	470.982	347.701	400.087	225.746	319.969	274.194	271.999
3	274.091	571.367	1006.693	424.380	392.884	257.476	237.752	360.684	244.439	335.460
4	294.915	249.775	811.850	434.289	432.736	337.362	243.002	397.269	265.436	369.143
5	322.229	255.158	572.306	452.744	469.366	260.237	262.365	459.043	287.421	306.854
6	346.989	273.125	547.876	92189.677	497.252	277.130	278.337	475.963	278.051	336.325
7	299.367	265.497	546.477	105921.365	278.489	301.152	303.726	291.662	305.337	369.874
STEP NO.					IMPROVEMENT RATIO					
1	.070	.988	.112	.176	.394	.311	.403	1.300	.958	.961
2	.083	.879	.537	.180	.343	.296	.469	.620	.685	.465
3	.085	1.193	.171	.162	.389	.189	.494	.700	.608	.576
4	.092	.514	.136	.166	.428	.249	.505	.771	.662	.634
5	.101	.525	.097	.173	.465	.191	.540	.893	.717	.525
6	.109	.563	.093	35.630	.493	.203	.579	.926	.693	.576
7	.093	.588	.093	40.988	.273	.221	.635	.562	.762	.635
STEP NO.					MINIMIZATION FUNCTION					
0	9.396	6.232	12.902	9.176	7.596	11.704	4.446	6.672	8.472	5.595
1	5.249	4.553	7.005	5.828	5.068	6.788	3.406	4.403	5.284	3.671
2	4.676	4.591	479.244	5.876	4.529	5.039	2.745	4.191	4.337	3.369
3	3.950	15.215	65.186	4.593	3.568	3.987	2.324	3.119	4.179	2.293
4	3.416	11.836	60.962	4.765	3.053	3.496	2.143	3.200	2.528	2.208
5	3.376	3.732	57.306	4.923	3.332	2.156	1.226	2.877	2.182	1.811
6	3.016	2.657	53.034	**********	3.362	2.083	1.591	2.913	1.964	1.838
7	2.216	2.667	51.006	646269.875	1.346	1.850	1.502	1.979	2.211	2.150

Table 15. Experimental Design Data for N=4, k=2, M=4, $\beta_{ij}/\sigma=20$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	.103	.300	.921	.837	1.495	4.474	2.073	2.362	1.624	.833
1	4.002	8.181	6.391	7.224	7.820	7.107	9.265	12.427	7.999	7.272
2	7.346	11.431	21.258	14.441	11.543	6.989	12.126	16.781	12.088	16.539
3	11.260	18.231	68.050	25.280	21.681	14.643	16.295	19.755	20.701	40.747
4	15.042	26.264	92.689	37.791	31.149	23.174	24.039	24.468	28.890	49.510
STEP NO.					AVERAGE VARIANCE					
0	39.906	23.867	5.385	5.718	4.582	2.929	4.085	4.724	4.437	5.738
1	3.807	3.076	3.647	3.601	3.196	3.183	2.864	2.611	3.095	3.599
2	3.733	3.291	2.703	3.252	3.430	3.539	3.152	2.808	3.265	3.172
3	3.854	3.201	2.226	3.029	3.061	3.445	3.320	3.099	3.075	2.498
4	4.086	3.212	2.245	2.939	3.061	3.359	3.308	3.295	3.119	2.653
STEP NO.					AVERAGE SQUARED BIAS					
0	10225.817	64302.469	7750.316	15971.041	4310.918	261.412	1469.428	4252.448	3067.603	16603.673
1	738.371	324.440	363.243	519.874	545.690	332.330	312.187	349.706	526.953	531.454
2	359.325	390.034	1284.002	524.938	440.385	393.484	364.155	358.978	411.518	1070.096
3	471.535	375.153	1249.549	487.965	519.994	401.008	451.576	411.857	500.680	646.605
4	452.527	446.269	1157.546	476.414	469.724	492.046	435.963	488.249	474.057	578.813
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	10265.723	64326.336	7755.700	15976.759	4315.500	264.341	1473.513	4257.172	3072.040	16609.411
1	742.177	327.516	366.890	523.476	548.886	335.513	315.051	352.318	530.048	535.053
2	363.057	393.325	1286.705	528.189	443.815	397.023	367.307	361.785	414.783	1073.268
3	475.389	378.354	1251.775	490.994	523.056	404.453	454.896	414.955	503.755	649.103
4	456.614	449.481	1159.791	479.353	472.784	495.405	439.271	491.544	477.176	581.466
STEP NO.					IMPROVEMENT RATIO					
1	.072	.005	.047	.033	.126	1.272	.212	.082	.172	.032
2	.035	.006	.165	.033	.102	1.508	.247	.084	.134	.064
3	.046	.006	.161	.030	.120	1.536	.307	.097	.163	.039
4	.044	.007	.149	.030	.109	1.884	.296	.115	.154	.035
STEP NO.					MINIMIZATION FUNCTION					
0	1.075	2.874	5.676	7.921	4.405	1.072	2.242	3.049	3.566	8.064
1	.595	1.145	2.668	4.097	1.944	.798	.553	1.085	1.430	4.191
2	.623	.945	21.175	3.005	1.458	.926	.405	.658	1.014	7.568
3	.752	.868	53.563	1.908	.759	1.012	.511	.589	.517	2.206
4	1.116	.609	13.304	1.240	.463	.827	.454	.739	.336	1.390

Table 16. Experimental Design Data for N=5, k=2, M=5, β_{ij}/σ=20

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	7.577	6.023	4.381	4.957	7.647	8.367	6.738	6.037	5.776	6.809
1	15.491	17.281	10.393	21.665	15.862	14.156	12.096	17.054	13.426	10.534
2	23.410	21.293	27.369	28.497	23.823	17.884	16.523	20.137	15.934	16.926
3	30.154	25.624	42.165	34.015	30.560	22.268	24.165	28.915	24.555	23.381
4	38.969	35.890	56.849	45.011	39.506	30.220	32.399	40.205	33.552	31.242
5	49.582	50.153	72.223	64.696	50.363	41.496	45.505	49.558	43.441	43.454
STEP NO.					AVERAGE VARIANCE					
0	3.168	3.328	4.411	3.655	3.158	2.948	3.258	3.866	3.378	3.259
1	2.946	2.815	4.186	2.660	2.924	2.965	3.144	2.857	3.049	3.345
2	2.947	3.074	3.010	2.861	2.932	3.195	3.290	3.153	3.367	3.264
3	3.086	3.304	2.890	3.095	3.075	3.399	3.309	3.138	3.287	3.340
4	3.171	3.275	2.889	3.134	3.158	3.461	3.389	3.135	3.333	3.422
5	3.246	3.233	2.933	3.015	3.229	3.484	3.344	3.247	3.401	3.413
STEP NO.					AVERAGE SQUARED BIAS					
0	1078.562	1733.645	564.833	5499.802	1146.143	308.235	285.609	653.944	594.958	275.128
1	397.300	363.090	936.285	563.835	405.156	329.037	343.044	329.547	303.752	356.685
2	445.954	374.816	442.781	529.211	450.452	382.751	411.382	354.825	364.528	387.361
3	449.911	411.645	427.392	503.608	453.922	459.650	433.994	403.174	425.226	441.217
4	516.267	467.593	496.455	504.707	518.963	487.796	476.148	454.907	468.648	495.900
5	544.916	521.800	519.410	537.641	544.966	539.154	556.931	510.213	536.747	516.663
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	1081.730	1736.973	569.244	5503.457	1149.301	311.182	288.867	657.810	598.336	278.387
1	400.246	365.905	940.470	566.495	408.081	332.002	346.188	332.404	306.801	360.030
2	448.900	377.890	445.791	532.072	453.384	385.946	414.672	357.978	367.895	390.625
3	452.996	414.949	430.283	506.703	456.997	463.048	437.303	406.313	428.513	444.557
4	519.437	470.868	499.345	507.841	522.121	491.257	479.537	458.042	471.981	499.322
5	548.162	525.033	522.343	540.656	548.196	542.638	560.275	513.459	540.148	520.076
STEP NO.					IMPROVEMENT RATIO					
1	.368	.209	1.656	.102	.353	1.067	1.201	.502	.510	1.297
2	.413	.216	.781	.096	.392	1.242	1.440	.541	.612	1.408
3	.416	.237	.754	.091	.395	1.493	1.519	.615	.714	1.603
4	.478	.269	.876	.092	.452	1.584	1.667	.694	.787	1.802
5	.505	.300	.916	.098	.475	1.751	1.949	.778	.901	1.877
STEP NO.					MINIMIZATION FUNCTION					
0	2.235	2.965	8.385	7.122	2.378	.693	1.013	2.231	1.719	.854
1	1.109	.699	6.017	2.940	1.169	.207	.655	.794	.584	.772
2	.579	.425	4.501	1.994	.622	.209	.656	.642	.671	.559
3	.431	.469	3.361	1.498	.456	.403	.774	.519	.637	.702
4	.353	.440	2.684	1.248	.363	.594	.740	.200	.487	.768
5	.437	.347	2.083	.694	.425	.713	.704	.359	.756	.911

Table 17. Experimental Design Data for N=8, k=2, M=5, $\beta_{ij}/\sigma=20$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	27.022	39.586	46.243	36.379	31.249	35.084	31.430	12.733	25.370	18.940
1	37.789	71.742	64.288	55.664	44.051	60.830	44.482	42.761	51.218	32.373
2	47.722	82.065	73.181	81.122	53.113	70.829	54.544	60.383	63.886	46.472
3	65.074	91.551	80.508	103.477	68.720	78.271	72.203	84.966	83.126	60.721
4	89.849	105.896	97.543	114.614	90.101	90.850	89.793	110.558	104.894	85.416
5	115.374	134.837	121.886	124.447	107.937	108.774	107.007	133.863	125.737	104.981
STEP NO.					AVERAGE VARIANCE					
0	3.180	2.861	2.743	2.886	3.035	2.951	3.029	4.314	3.262	3.725
1	3.199	2.631	2.722	2.853	3.067	2.736	3.069	3.153	2.921	3.397
2	3.290	2.791	2.886	2.784	3.191	2.883	3.169	3.130	3.029	3.352
3	3.270	2.958	3.074	2.805	3.205	3.067	3.152	3.032	3.027	3.359
4	3.195	3.063	3.129	2.951	3.191	3.182	3.193	3.002	3.040	3.249
5	3.184	3.035	3.130	3.113	3.263	3.247	3.268	3.039	3.093	3.292
STEP NO.					AVERAGE SQUARED BIAS					
0	601.081	728.849	631.815	454.252	508.439	745.489	566.868	3356.770	860.925	522.050
1	729.821	583.159	582.903	547.116	518.165	682.738	542.378	511.436	484.434	541.039
2	830.227	574.768	579.192	591.857	578.861	720.303	587.662	540.495	513.074	531.136
3	943.721	591.189	601.297	629.352	665.086	790.729	680.152	665.443	558.922	606.603
4	663.917	620.696	629.437	654.161	634.276	803.046	687.525	683.646	601.574	625.677
5	749.252	697.245	688.162	697.735	701.638	888.885	770.779	757.354	651.362	676.785
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	604.261	731.710	634.558	457.137	511.475	748.440	569.897	3361.084	864.187	525.775
1	733.021	585.789	585.625	549.969	521.232	685.474	545.447	514.590	487.355	544.436
2	833.518	577.558	582.077	594.641	582.052	723.186	590.831	543.625	516.103	534.488
3	946.991	594.147	604.371	632.157	668.291	793.796	683.304	668.475	561.950	609.963
4	667.112	623.759	632.566	657.112	637.467	806.228	690.719	686.648	604.614	628.925
5	752.436	700.280	691.292	700.848	704.902	892.132	774.046	760.394	654.455	680.077
STEP NO.					IMPROVEMENT RATIO					
1	1.214	.799	.922	1.205	1.019	.915	.957	.152	.562	1.036
2	1.382	.788	.915	1.303	1.139	.966	1.037	.161	.595	1.016
3	1.570	.810	.952	1.385	1.308	1.060	1.209	.198	.648	1.161
4	1.104	.851	.996	1.440	1.247	1.077	1.213	.203	.698	1.197
5	1.246	.956	1.089	1.536	1.380	1.192	1.360	.225	.755	1.295
STEP NO.					MINIMIZATION FUNCTION					
0	1.777	5.439	1.886	4.747	1.026	3.277	1.316	8.741	4.789	1.708
1	1.647	2.623	1.069	3.389	.589	1.487	.750	3.499	1.598	1.112
2	1.851	1.910	.655	2.216	.607	1.129	.750	2.411	1.013	.982
3	1.697	1.509	.520	1.549	.595	1.074	.540	1.474	.591	1.006
4	1.165	1.351	.577	1.292	.545	1.233	.535	.998	.258	.632
5	.941	.928	.343	1.304	.609	1.272	.679	.653	.153	.675

Table 18. Experimental Design Data for N=6, k=3, M=4, β_{ij}/σ=20

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	.443	.421	.513	1.545	.052	.365	.097	.038	.069	1.733
1	11.219	3.222	3.893	7.329	.816	3.459	.710	.159	.892	31.729
2	18.277	11.710	25.545	10.305	5.808	6.445	13.795	6.510	4.570	47.699
3	32.799	26.059	50.664	22.492	19.594	10.961	35.258	15.174	19.138	67.147
4	47.531	40.358	70.278	48.012	40.544	29.757	51.715	31.387	42.586	92.170
STEP NO.					AVERAGE VARIANCE					
0	24.650	11.930	30.874	7.970	35.215	15.364	83.305	69.482	32.629	11.195
1	4.991	8.967	11.949	6.743	18.811	7.008	37.879	74.144	17.533	3.690
2	4.909	5.670	4.612	7.374	8.271	6.964	5.590	7.227	10.051	3.854
3	4.575	4.968	4.114	6.161	5.747	7.161	4.567	6.549	5.975	3.995
4	4.614	4.858	4.177	4.962	4.961	5.272	4.617	5.529	4.930	4.062
STEP NO.					AVERAGE SQUARED BIAS					
0	49712.562	7332.508	1419.666	2330.877	7173.616	3084.084	6593.752	2546.888	5519.621	122599.954
1	922.387	1146.424	7863.943	539.837	982.231	867.720	31171.877	14706.866	1373.321	868.460
2	1063.868	1053.092	805.356	647.883	1735.905	874.841	943.750	1045.320	2218.617	774.548
3	1224.510	1231.062	1062.114	816.407	1199.339	606.223	968.627	849.888	1486.201	795.495
4	1342.964	835.990	1039.867	902.343	802.894	749.446	1021.226	816.968	846.544	775.222
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	49737.212	7344.437	1450.540	2338.846	7208.831	3099.448	6677.057	2616.370	5552.250	122611.148
1	927.378	1155.390	7875.892	546.580	1001.042	874.728	31209.757	14781.010	1390.854	872.150
2	1068.777	1058.762	809.968	655.257	1744.176	881.805	949.340	1052.546	2228.668	778.403
3	1229.086	1236.029	1066.227	822.467	1205.086	613.384	973.193	856.437	1492.177	799.480
4	1347.578	840.848	1044.044	907.305	807.855	754.719	1025.843	822.497	851.473	779.284
STEP NO.					IMPROVEMENT RATIO					
1	.019	.157	5.445	.232	.138	.281	4.677	5.658	.250	.007
2	.021	.144	.557	.279	.241	.283	.141	.401	.401	.006
3	.025	.168	.734	.350	.167	.196	.145	.326	.268	.006
4	.027	.114	.718	.386	.111	.242	.153	.313	.152	.006
STEP NO.					MINIMIZATION FUNCTION					
0	3.718	5.242	6.330	9.169	5.028	2.601	5.330	5.810	5.327	13.010
1	1.995	2.801	4.806	4.555	3.508	1.808	3.464	3.050	3.675	7.705
2	1.980	2.665	3.795	3.886	3.231	2.262	2.966	2.643	3.487	6.087
3	1.746	1.870	3.052	3.318	2.702	2.212	1.939	1.845	2.883	5.100
4	1.827	1.830	2.802	2.717	2.211	2.100	1.782	2.011	2.335	4.158

Table 19. Experimental Design Data for N=8, k=3, M=5, $\beta_{ij}/\sigma=20$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	4.474	9.431	8.936	18.169	18.885	7.605	17.021	4.977	2.895	1.330
1	23.216	44.205	29.414	68.r77	76.735	41.551	74.273	19.358	13.493	7.336
2	53.396	72.325	60.655	95.766	110.619	56.518	108.068	47.368	42.532	18.942
3	86.731	108.938	148.778	130.807	146.641	98.237	144.568	82.418	77.777	36.273
4	112.530	138.968	178.627	163.192	180.646	148.830	178.215	105.846	102.414	74.217
5	146.552	180.490	232.431	192.312	208.199	186.144	204.458	138.055	158.148	100.150
STEP NO.					AVERAGE VARIANCE					
0	8.644	6.638	6.421	5.180	5.226	7.364	5.376	7.797	9.010	13.458
1	5.555	4.434	5.570	3.851	3.762	4.647	3.800	5.992	7.507	7.229
2	4.578	4.286	4.740	3.899	3.776	4.761	3.813	4.692	5.236	6.358
3	4.369	4.174	3.844	3.936	3.848	4.287	3.881	4.398	4.822	5.557
4	4.468	4.264	4.003	4.038	3.957	4.127	3.994	4.517	4.922	4.964
5	4.497	4.314	4.047	4.192	4.127	4.217	4.173	4.557	4.636	5.028
STEP NO.					AVERAGE SQUARED BIAS					
0	3135.044	2720.417	2757.926	2751.199	4322.737	10761.395	5746.045	5350.034	2900.989	1042.669
1	969.366	861.808	1327.545	685.387	819.296	725.172	757.273	2071.833	1109.963	1285.643
2	823.320	704.929	2122.414	722.826	839.461	691.117	762.391	1873.698	747.255	1128.691
3	715.434	799.912	886.963	725.314	833.340	775.073	764.063	899.280	846.512	1610.424
4	826.975	815.464	966.431	788.288	883.352	763.609	801.835	1018.127	963.211	962.274
5	890.025	936.537	916.778	843.042	939.058	835.945	855.592	1132.499	936.739	853.067
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	3143.688	2727.054	2764.347	2756.379	4327.963	10768.759	5751.422	5357.831	2909.999	1056.127
1	974.921	866.242	1333.115	689.238	823.058	729.819	761.074	2077.824	1117.470	1292.872
2	827.898	709.214	2127.154	726.725	843.237	695.878	766.204	1878.391	752.491	1135.050
3	719.803	804.086	890.807	729.250	837.188	779.359	767.944	903.679	851.335	1615.982
4	831.443	819.728	970.434	792.327	887.309	767.736	805.829	1022.644	968.133	967.238
5	894.522	940.850	920.824	847.235	943.185	840.161	859.765	1137.056	941.375	858.096
STEP NO.					IMPROVEMENT RATIO					
1	.309	.316	.481	.249	.189	.067	.132	.387	.383	1.225
2	.262	.259	.769	.262	.194	.064	.132	.350	.257	1.075
3	.228	.293	.321	.263	.192	.072	.133	.168	.291	1.532
4	.263	.299	.350	.286	.204	.071	.139	.190	.331	.915
5	.283	.343	.332	.306	.217	.077	.149	.211	.322	.811
STEP NO.					MINIMIZATION FUNCTION					
0	6.794	8.889	11.821	6.544	8.158	6.709	9.003	5.233	12.481	3.314
1	4.238	4.989	7.778	2.946	4.039	3.438	4.425	2.971	7.149	3.484
2	3.272	3.925	9.477	2.173	3.031	3.200	3.359	2.588	5.717	2.584
3	2.547	3.095	5.137	1.676	2.378	2.776	2.609	1.649	4.271	3.038
4	2.588	2.973	4.627	1.369	1.979	2.252	2.196	1.782	4.020	2.022
5	2.783	2.806	3.804	1.373	1.909	2.192	2.105	1.976	3.889	2.253

Table 20. Experimental Design Data for N=10, k=3, M=7, $\beta_{ij}/\sigma=20$

TEST CASE	1	2	3	4	5	6	7	8	9	10
STEP NO.					DETERMINANT OF THE (X X) MATRIX					
0	8.824	11.062	.763	3.774	6.781	10.872	22.997	6.679	8.310	11.477
1	51.881	26.698	5.269	29.125	30.230	48.452	67.822	35.469	21.731	41.284
2	96.822	64.468	105.697	55.894	72.972	68.285	108.594	81.165	49.425	101.064
3	193.797	128.734	258.152	128.492	127.495	115.479	148.890	129.344	95.696	168.051
4	257.430	304.540	540.603	160.583	162.672	213.017	223.950	160.865	214.875	212.635
5	301.352	378.132	960.229	224.903	227.699	322.513	331.962	241.533	288.331	303.129
6	408.142	544.506	1248.320	9014.792	297.236	403.556	391.225	313.702	379.297	366.848
7	545.334	695.342	1444.869	40393.281	478.625	518.174	478.559	455.287	479.775	439.149
STEP NO.					AVERAGE VARIANCE					
0	11.692	8.291	30.829	12.786	9.131	7.275	6.742	11.429	7.801	8.872
1	6.022	7.438	21.577	6.632	6.370	5.662	4.838	6.047	7.224	5.977
2	5.005	5.599	6.223	5.597	5.000	5.580	4.644	4.915	6.586	4.627
3	4.253	4.756	5.571	4.638	4.663	5.148	4.649	4.707	5.407	4.358
4	4.226	4.170	4.240	4.743	4.759	4.486	4.391	4.816	4.423	4.425
5	4.362	4.225	3.680	4.690	4.685	4.263	4.223	4.599	4.390	4.312
6	4.277	4.013	3.603	3.501	4.668	4.304	4.322	4.611	4.363	4.394
7	4.218	3.981	3.667	2.625	4.358	4.276	4.360	4.413	4.352	4.458
STEP NO.					AVERAGE SQUARED BIAS					
0	12527.208	1884.725	23238.891	10317.319	3968.177	5318.241	1871.865	2004.307	1558.409	2276.172
1	879.712	1865.785	2544.292	1821.435	1565.137	1655.234	764.262	2635.562	1496.076	2200.221
2	1049.378	1667.822	12522.888	1861.542	1370.805	1578.029	884.366	1260.216	1070.433	1069.489
3	1078.994	2266.446	4004.486	1678.968	1552.884	1009.312	932.410	1423.909	956.128	1324.407
4	1162.754	982.418	3230.440	1718.183	1711.909	1331.502	954.445	1569.811	1044.051	1458.870
5	1271.467	1003.736	2274.480	1792.215	1858.727	1023.896	1032.567	1817.775	1132.125	1210.168
6	1370.687	1076.450	2177.093	368740.707	1970.337	1091.304	1096.061	1885.406	1094.752	1327.722
7	1180.595	1126.023	2171.237	423674.965	1096.521	1187.504	1197.463	1149.076	1203.938	1461.666
STEP NO.					MINIMUM MEAN SQUARE ERROR					
0	12538.900	1893.016	23269.720	10330.104	3977.308	5325.517	1878.607	2015.736	1566.210	2285.044
1	885.735	1873.223	2565.869	1828.066	1571.506	1660.896	769.100	2641.609	1503.300	2206.198
2	1054.383	1673.421	12529.111	1867.139	1375.805	1583.609	889.014	1265.131	1077.018	1074.116
3	1083.247	2271.201	4010.058	1683.606	1557.547	1014.460	937.059	1428.616	961.535	1328.765
4	1166.980	986.589	3234.680	1722.926	1716.668	1335.988	958.836	1574.628	1048.474	1463.295
5	1275.829	1007.960	2278.160	1796.905	1863.411	1028.159	1036.790	1822.374	1136.516	1214.480
6	1374.964	1080.463	2180.690	368744.207	1975.005	1095.608	1100.383	1890.017	1099.115	1332.116
7	1184.813	1130.004	2174.904	423677.586	1100.879	1191.780	1201.823	1153.489	1208.291	1466.124
STEP NO.					IMPROVEMENT RATIO					
1	.070	.989	.110	.177	.394	.311	.409	1.311	.960	.965
2	.084	.883	.538	.180	.345	.297	.472	.626	.686	.469
3	.086	1.200	.172	.162	.391	.190	.497	.709	.612	.580
4	.093	.519	.139	.166	.431	.250	.509	.789	.668	.639
5	.101	.531	.099	.173	.468	.192	.550	.903	.724	.530
6	.109	.569	.093	35.715	.496	.205	.584	.937	.700	.582
7	.094	.595	.093	41.035	.276	.223	.638	.571	.770	.640
STEP NO.					MINIMIZATION FUNCTION					
0	9.306	6.832	12.902	9.136	7.598	11.704	4.446	6.672	8.472	5.595
1	5.249	4.553	7.905	5.538	5.068	6.788	3.406	4.403	5.284	3.671
2	4.620	4.521	479.244	5.676	4.529	5.039	2.745	4.191	4.337	3.369
3	3.950	15.215	65.186	4.523	3.568	3.987	2.324	3.117	4.179	2.293
4	3.410	11.036	60.802	4.765	3.653	3.496	2.145	3.260	2.528	2.209
5	3.396	3.732	57.308	4.423	3.332	2.158	1.229	2.877	2.182	1.811
6	3.016	2.607	53.834	**********	3.362	2.083	1.391	2.313	1.964	1.838
7	2.216	2.067	51.406	462608.875	1.348	1.850	1.502	1.979	2.211	2.150

APPENDIX D

DEVELOPMENT OF THE MOMENT MATRIX AND PRECISION MATRIX

The moment matrix is defined to be

$$N^{-1}\underline{X}'\underline{X}$$

where N is the total number of experimental runs in the design. In the first order case

$$N^{-1}\underline{X}'\underline{X} = \frac{1}{N}\begin{bmatrix} 1, x_1, x_2, \ldots, x_k \end{bmatrix}\begin{bmatrix} 1 \\ x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_k \end{bmatrix}$$

$$= \begin{array}{c|c} & \begin{matrix} 1 & x_1 & x_2 & \cdots & x_k \end{matrix} \\ \begin{matrix} 1 \\ x_1 \\ x_2 \\ \vdots \\ x_k \end{matrix} & \begin{bmatrix} 1 & [1] & [2] & \cdots & [k] \\ & [11] & [12] & \cdots & [1k] \\ & & [22] & \cdots & [2k] \\ & \text{sym} & & & \vdots \\ & & & & [kk] \end{bmatrix} \end{array}$$

where

$$[ij]=\frac{1}{N}\sum_{u=1}^{N} x_{iu}x_{ju}$$

(called second order moments)

and

$$[i]=\frac{1}{N}\sum_{u=i}^{N} x_{iu}\ .$$

(called first order moments)

Using the usual scaling convention

$$\sum_{u=1}^{N} x_{iu}=0 \qquad \text{and} \qquad \sum_{u=1}^{N} x_{iu}^{2}=N$$

the moment matrix now reduces to

$$N^{-1}\underline{X}'\underline{X}=\begin{array}{c|c} & \begin{array}{cccccc} 1 & x_1 & x_2 & \cdots & & x_k \end{array} \\ \begin{array}{c} 1 \\ x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ x_k \end{array} & \left[\begin{array}{cccccc} 1 & 0 & 0 & & & 0 \\ & 1 & [12] & \cdots & & [1k] \\ & & 1 & \cdots & & [2k] \\ & & & & & \vdots \\ \text{sym} & & & & & [k-1,k] \\ & & & & & 1 \end{array}\right] \end{array}$$

Now consider the second order model with k=2:

$$N^{-1}\underline{X}'\underline{X}=\begin{array}{c|cccccc|}
 & 1 & x_1 & x_2 & x_1^2 & x_2^2 & x_1x_2 \\
\hline
1 & 1 & 0 & 0 & 1 & 1 & [12] \\
x_1 & & 1 & [12] & [111] & [122] & [112] \\
x_2 & & & 1 & [112] & [222] & [122] \\
x_1^2 & & & & [1111] & [1122] & [1112] \\
x_2^2 & \text{sym} & & & & [2222] & [1222] \\
x_1x_2 & & & & & & [1122]
\end{array}$$

where fourth order moments are of the type

$$[1111]=1/N\sum_{u=1}^{N}x_{1u}^4$$

$$[1122]=1/N\sum_{u=1}^{N}x_{1u}^2x_{2u}^2$$

$$[1112]=1/N\sum_{u=1}^{N}x_{1u}^3x_{2u} \quad .$$

The inverse of the moment matrix is the precision matrix. That is,

$$C=[1/N(\underline{X}'\underline{X})]^{-1}$$

$$C=(\underline{X}'\underline{X})^{-1}N.$$

APPENDIX E

SAMPLE ESTIMATE OF THE STARTING VALUE FOR NEWTON'S METHOD

Randomly selected design points within an unit sphere of interest are assumed to be:

x_1	x_2	x_3
0	-.8	0
-.8	.5	-.3
-.9	0	.3
.5	-.3	-.5
-.5	-.4	-.5

and

$$\sum_{u=1}^{5} x_{u1} = -1.7 \qquad \sum_{u=1}^{5} x_{u2} = -1.0 \qquad \sum_{u=1}^{5} x_{u3} = -1.0.$$

The new observation is added to the orthant necessary to maintain balance, that is the new observation must be in orthant (+++). Since the value of $G = \pm\sqrt{1/k+2}$ or .46, the new observation is added at (.46,.46,.46). Now the iterative solution technique is applied to the above initial experiment with the designated augmented observation.

When this augmented observation is optimally located, it is incorporated into the above design, and the estimation process is repeated for the next observation to be added. This sequential augmentation technique is continued until all of the M allowable observations are added to the initial experiment.

APPENDIX F

FORTRAN PROGRAM

```
C       COMPUTER-AIDED DESIGN OF EXPERIMENTS
C       NEWTON S METHOD OF NUMERICAL ANALSIS
        DIMENSION ERAT(5,5,5),ERATA(5,5,5)
        DIMENSION DA(100,10)
        DIMENSION DM(100,10) ,COLT(10),AUGP(10,10),OMM1(10),OMM2(10)
        DIMENSION OMM3(10),AUGM1(10),AUGM2(10),AUGM3(10),FUN(10,10),JC(20)
        DIMENSION TERA(10,10)
        DIMENSION OOM4(100),OOMA4(100)
        DIMENSION PFUN(10,10,10,10),AJ(100,100),A(100,100)
        DIMENSION XTX(11,11),XTXI(11,11),XATXA(11,11),XATXAI(11,11),V(2)
        DIMENSION YDET(10,10),YV(10,10),YB(10,10),YCJ(10,10),YRI(10,10),
       1YF(10,10)
 1010   FORMAT (4I2)
 1020   FORMAT (1H1,10X,'DESIGN MATRIX, TEST CASE--',I3)
 1030   FORMAT (/10X,10E10.3)
 1040   FORMAT (/10X,'AUGMENTED MATRIX, TEST CASE--',I3)
 1080   FORMAT (/10X,'FAILED TO CONVERGE IN 20 ITERATIONS')
 1015   FORMAT(/5X,'TEST CASE--',I3,5X,'N=',I2,2X,'K=',I1,2X,'M=',I2,2X,'S
       1TEP NO. ',I2)
 1090   FORMAT (//10X,'DETERMINATE OF THE X X MATRIX-- ',E10.3/10X,
       1'DETERMINATE OF THE XA XA MATRIX--',E10.3)
 1100   FORMAT (//10X,'ESTIMATED J-VALUE OF ORIGINAL MATRIX-- ',E15.8/10X,
       1'ESTIMATED J-VALUE OF AUGMENTED MATRIX--',E15.8/10X,
       2'IMPROVEMENT RATIO--',E15.8)
 1110   FORMAT(//10X,'ERROR RETURN-CONDITION',I3,'PROCEED TO NEXT TEST')
 1120   FORMAT(//10X,'FAILURE TO CONVERGE INITIAL ESTIMATES INSUFFCIENT')
        LFY=0
        READ(5,1000) NH
 1000   FORMAT (I3)
        MH=0
```

```
    1 READ(5,1010) N,K,M,IT
      MM=M
      DO 102 I2=1,IT
      CALL RANMA (DM,N,K,LFY,YFL)
      WRITE(6,1020) I2
      DO 5 I=1,N
    5 WRITE(6,1030) (DM(I,J),J=1,K)
      DO 101 MI=1,MM
      MI1=MI+1
      WRITE(6,1015) I2,N,K,MM,MI
      M=1
      K1=0
      DO 6 I=1,K
    6 COLT(I)=0.0
      DO 10 J=1,K
      DO 10 I=1,N
      COLT(J)=DM(I,J)+COLT(J)
   10 CONTINUE
      DO 14 J=1,K
C*  THE TEST FOR EQUALITY BETWEEN NON-INTEGERS MAY NOT BE MEANINGFUL.
      IF(COLT(J).EQ.0) GO TO 13
      GO TO 14
   13 COLT(J)=0.0001
   14 CONTINUE
      G=SQRT(1.0/(K+2))
      DO 15 I=1,M
      DO 15 J=1,K
      AJGP(I,J)=G*(COLT(J)/(ABS(COLT(J))))*(-1.0)
   15 CONTINUE
      DO 150 I=1,M
      DO 150 J=1,K
      DO 150 L1=1,M
      DO 150 L2=1,K
      PFUN(I,J,L1,L2)=0
```

```
  150 CONTINUE
      DO 153 J1=1,K
      DO 153 J2=J1,K
      DO 153 J3=J2,K
      ERAT(J1,J2,J3)=0.0
  153 CONTINUE
      DO 20 I=1,K
      OMM1(I)=0.0
      OMM2(I)=(-1.0*(N+M)/(K*2))
      OMM3(I)=0.0
   20 CONTINUE
      DO 24 J=1,K
      DO 24 I=1,N
      OMM1(J)=COLT(J)
      OMM2(J)=(OMM2(J)+(DM(I,J)**2))
      OMM3(J)=OMM3(J)+(DM(I,J)**3)
   24 CONTINUE
      DO 155 J1=1,K
      DO 155 J2=J1,K
      DO 155 J3=J2,K
      DO 155 I=1,N
      ERAT(J1,J2,J3)=ERAT(J1,J2,J3)+(DM(I,J1)*DM(I,J2)*DM(I,J3))
  155 CONTINUE
    2 CONTINUE
   25 DO 56 I1=1,21
      DO 26 I=1,K
      AUGM1(I)=0.0
      AUGM2(I)=0.0
      AUGM3(I)=0.0
   26 CONTINUE
      DO 158 J1=1,K
      DO 158 J2=J1,K
      DO 158 J3=J2,K
```

```
      ERATA(J1,J2,J3)=0.0
  158 CONTINUE
      DO 30 J=1,K
      DO 30 I=1,M
      AUGM1(J)=AUGM1(J)+AUGP(I,J)
      AUGM2(J)=AUGM2(J)+(AUGP(I,J)**2)
      AUGM3(J)=AUGM3(J)+(AUGP(I,J)**3)
   30 CONTINUE
      DO 160 J1=1,K
      DO 160 J2=J1,K
      DO 160 J3=J2,K
      DO 160 I=1,M
      ERATA(J1,J2,J3)=ERATA(J1,J2,J3)+(AUGP(I,J1)*AUGP(I,J2)*AUGP(I,J3))
  160 CONTINUE
      DO 225 I=1,M
      DO 225 J=1,K
      TERA(I,J)=0
  225 CONTINUE
      K4=K-1
      DO 250 I=1,M
      DO 250 J=1,K
      DO 250 J1=1,K4
      DO 250 J2=J1,K
      J4=J2
      IF(J2.EQ.J1) J4=J4+1
      DO 250 J3=J4,K
      XST=2.0
      IF(J3.EQ.J) GO TO 245
      IF(J2.EQ.J) GO TO 246
      IF(J1.EQ.J) GO TO 247
      TERA(I,J)=TERA(I,J)+0.0
      GO TO 250
  245 IF(J3.EQ.J2) XST=4.0
      GO TO 248
```

```
 246 IF(J2.EQ.J1) XST=4.0
     GO TO 249
 247 TERA(I,J)=TERA(I,J)+((ERAT(J1,J2,J3)+ERATA(J1,J2,J3))*(AUGP(I,J2)*
    1AUGP(I,J3)*XST))
     GO TO 250
 248 TERA(I,J)=TERA(I,J)+((ERAT(J1,J2,J3)+ERATA(J1,J2,J3))*(AUGP(I,J1)*
    1AUGP(I,J2)*XST))
     GO TO 250
 249 TERA(I,J)=TERA(I,J)+((ERAT(J1,J2,J3)+ERATA(J1,J2,J3))*(AUGP(I,J1)*
    1AUGP(I,J3)*XST))
 250 CONTINUE
     DO 430 I=1,M
     DO 430 J=1,K
     DO 430 L3=1,K
     DO 430 L4=1,N
     IF (L3.EQ.J) GO TO 430
     TERA(I,J)=TERA(I,J)+2.0*AUGP(I,L3)*(DM(L4,L3)*DM(L4,J)+AUGP(L4,L3)
    1*AUGP(L4,J))
 430 CONTINUE
     DO 31 J=1,K
     DO 31 I=1,M
     FUN(I,J)=2*(OMM1(J)+AUGM1(J))+4*(OMM2(J)+AUGM2(J))*AUGP(I,J)
    1+6*(OMM3(J)+AUGM3(J))*(AUGP(I,J)**2)+TERA(I,J)
  31 CONTINUE
     TFUN=0.0
     DO 34 I=1,M
     DO 34 J=1,K
  34 TFUN=TFUN+ABS(FUN(I,J))
     IF ((ABS(TFUN)).LT.1.E-5) GO TO 65
     DO 36 I=1,M
     DO 36 J=1,K
     DO 36 L1=1,M
     DO 36 L2=1,K
```

```
      IF(L1.EQ.I.AND.L2.EQ.J) GO TO 35
      IF (L2.EQ.J) GO TO 37
      PFUN(I,J,L1,L2)=0.0
      GO TO 36
   37 PFUN(I,J,L1,L2)=2+(8*AUGP(I,J)*AUGP(L1,L2))+18*(AUGP(I,J)**2)
     1*(AUGP(L1,L2)**2)
      GO TO 36
   35 PFUN(I,J,L1,L2)=2+(4*(OMM2(J)+AUGM2(J)))+12*AUGP(I,J)
     1*(OMM3(J)+AUGM3(J))+8*(AUGP(I,J)**2)+18*(AUGP(I,J)**4)
   36 CONTINUE
      DO 450 I=1,M
      DO 450 J=1,K
      DO 450 J1=1,M
      DO 450 J2=1,K
      DO 450 J3=1,M
      DO 450 J4=1,K
      XST=2.0
      IF(J1.EQ.I.AND.J2.EQ.J) GO TO 446
      IF(J3.EQ.J1.AND.J4.EQ.J2) XST=4.0
      IF(J3.EQ.I.AND.J4.EQ.J) XST=4.0
      PFUN(I,J,J1,J2)=PFUN(I,J,J1,J2)+(XST*(AUGP(J1,J2)*(AUGP(J3,J4)**2)
     1*AUGP(I,J)))
      GO TO 450
  446 DO 449 J5=J4,K
      IF(J4.EQ.J2.AND.J5.EQ.J4) GO TO 449
      IF(J3.EQ.J1.AND.J4.EQ.J2) XST=8.0
      IF(J3.EQ.J1.AND.J5.EQ.J2) XST=8.0
      PFUN(I,J,J1,J2)=PFUN(I,J,J1,J2)+(XST*(AUGP(J3,J4)**2)*(AUGP(J3,J5)
     1**2))
  449 CONTINUE
  450 CONTINUE
      K4=K-1
      DO 470 I=1,M
      DO 470 J=1,K
```

```
      DO 470 J1=1,M
      DO 470 J2=1,K
      J7=0
      DO 470 J3=1,K4
      DO 470 J4=J3,K
      J6=J4
      IF(J4.EQ.J3) J6=J5+1
      DO 470 J5=J6,K
      XST=2.0
      IF(J5.EQ.J2.AND.J4.EQ.J) GO TO 461
      IF(J4.EQ.J2.AND.J3.EQ.J) GO TO 461
      IF(J5.EQ.J2.AND.J3.EQ.J) GO TO 461
      IF(J5.EQ.J.AND.J4.EQ.J2) GO TO 461
      IF(J5.EQ.J.AND.J3.EQ.J2) GO TO 461
      PFUN(I,J,J1,J2)=PFUN(I,J,J1,J2)+0.0
      GO TO 470
  461 J7=J7+1
      IF(J1.EQ.I.AND.J2.EQ.J) GO TO 462
      IF(J7.EQ.J.OR.J7.EQ.J2) XST=4.0
      PFUN(I,J,J1,J2)=PFUN(I,J,J1,J2)+(XST*AUGP(J1,J7)*(ERAT(J3,J4,J5)+
     1ERATA(J3,J4,J5)))
      GO TO 470
  462 XST=4.0
      IF(J7.EQ.J2) GO TO 461
      PFUN(I,J,J1,J2)=PFUN(I,J,J1,J2)+(XST*AUGP(J1,J7)*(ERAT(J3,J4,J5)+
     1ERATA(J3,J4,J5)))
  470 CONTINUE
      DO 530 I=1,M
      DO 530 J=1,K
      DO 530 L1=1,M
      DO 530 L2=1,K
      IF (L1.EQ.I.AND.L2.EQ.J) GO TO 505
      IF (L1.EQ.I) GO TO 510
```

```
      IF (L2.EQ.J) GO TO 515
      PFUN(I,J,L1,L2)=PFUN(I,J,L1,L2)+2.0*AUGP(I,L2)*AUGP(L1,J)
      GO TO 530
  505 DO 506 L3=1,K
      IF (L3.EQ.L2) GO TO 506
      PFUN(I,J,L1,L2)=PFUN(I,J,L1,L2)+2.0*(AUGP(L1,L3)**2)
  506 CONTINUE
      GO TO 530
  510 PFUN(I,J,L1,L2)=PFUN(I,J,L1,L2)+2.0*AUGP(I,J)*AUGP(L1,L2)
      DO 511 L4=1,N
      PFUN(I,J,L1,L2)=PFUN(I,J,L1,L2)+2.0*(DM(L4,J)*DM(L4,L2)+
     1AUGP(L4,J)*AUGP(L4,L2))
  511 CONTINUE
      GO TO 530
  515 DO 516 L3=1,K
      IF (L3.EQ.L2) GO TO 516
      PFUN(I,J,L1,L2)=PFUN(I,J,L1,L2)+2.0*AUGP(I,L3)*AUGP(L1,L3)
  516 CONTINUE
  530 CONTINUE
      L3=0
      DO 40 I=1,M
      DO 40 J=1,K
      L3=L3+1
      L4=0
      DO 40 L1=1,M
      DO 40 L2=1,K
      L4=L4+1
      AJ(L3,L4)=PFUN(I,J,L1,L2)
   40 CONTINUE
      N1=M*K
      MC=M*K
      V(1)=2
      CALL GJR(AJ,100,100,N1,MC,$70,JC,V)
```

```
      DETJ=V(1)*EXP(V(2))
      DO 55 L5=1,M
      DO 55 L6=1,K
      DET=0
      L3=0
      DO 50 I=1,M
      DO 50 J=1,K
      L3=L3+1
      L4=0
      DO 50 L1=1,M
      DO 50 L2=1,K
      L4=L4+1
      IF(L1.EQ.L5 .AND. L2.EQ.L6)GO TO 45
      A(L3,L4)=PFUN(I,J,L1,L2)
      GO TO 50
   45 A(L3,L4)=-1.0*FUN(I,J)
   50 CONTINUE
      V(1)=2
      CALL GJR(A,100,100,N1,MC,$54,JC,V)
      DET=V(1)*EXP(V(2))
      AUGP(L5,L6)=AUGP(L5,L6)+(DET/DETJ)
      GO TO 55
   54 WRITE(6,1110) JC(1)
   55 CONTINUE
   56 CONTINUE
   65 CALL XMA(DM,AUGP,XTX,XTXI,XATXA,XATXAI,DETX,DETXA,N,K,M,DA)
      IF (MI.EQ.1) GO TO 63
      GO TO 64
   63 XDETX=DETX
   64 WRITE(6,1090) XDETX,DETXA
      YDET(1,I2)=XDETX
      YDET(MI1,I2)=DETXA
      CALL CKR(CJ,CJA,RI,XTX,XTXI,XATXA,XATXAI,N,K,M,DM,DA,MI,I2,YV,YB)
      IF (MI.EQ.1) GO TO 61
```

```
      GO TO 62
   61 XCJ=CJ
   62 WRITE(6,1100)XCJ,CJA,RI
      YCJ(1,I2)=XCJ
      YCJ(MI1,I2)=CJA
      YRI(MI,I2)=RI
      OOM1=0
      OOM2=0
      OOM3=0
      OOM5=0
      OOMA1=0
      OOMA2=0
      OOMA3=0
      OOMA5=0
      DO 66 I=1,K
      OOM1=OOM1+(OMM1(I)**2)
      OOM2=OOM2+((OMM2(I)+(1.0*(N+M)/(K+2))-(1.0*N/(K+2)))**2)
      OOM3=OOM3+(OMM3(I)**2)
      OOMA1=OOMA1+((OMM1(I)+AUGM1(I))**2)
      OOMA2=OOMA2+((OMM2(I)+AUGM2(I))**2)
      OOMA3=OOMA3+((OMM3(I)+AUGM3(I))**2)
   66 CONTINUE
      K1=K-1
      L1=0
      DO 80 J=1,K1
      J1=J+1
      DO 80 L3=J1,K
      L1=L1+1
      OOM4(L1)=0
      OOMA4(L1)=0
   80 CONTINUE
      K1=K-1
      L1=0
```

```
      DO 68 J=1,K1
      J1=J+1
      DO 68 L3=J1,K
      L1=L1+1
      DO 67 L4=1,N
      OOM4(L1)=OOM4(L1)+DM(L4,J)*DM(L4,L3)
   67 CONTINUE
      OOM5=OOM5+OOM4(L1)**2
   68 CONTINUE
      K1=K-1
      L1=0
      DO 71 J=1,K1
      J1=J+1
      DO 71 L3=J1,K
      L1=L1+1
      DO 69 L4=1,M
      OOMA4(L1)=OOMA4(L1)+AUGP(L4,J)*AUGP(L4,L3)
   69 CONTINUE
      OOMA5=OOMA5+(OOM4(L1)+OOMA4(L1))**2
   71 CONTINUE
      OOM6=0
      OOMA6=0
      K4=K-1
      DO 610 I=1,M
      DO 610 J=1,K
      DO 610 J1=1,K4
      DO 610 J2=J1,K
      J4=J2
      IF(J2.EQ.J1) J4=J4+1
      DO 610 J3=J4,K
      OOM6=OOM6+(ERAT(J1,J2,J3)**2)
      OOMA6=OOMA6+((ERAT(J1,J2,J3)+ERATA(J1,J2,J3))**2)
  610 CONTINUE
      FUNIM=OOM1+OOM2+OOM3+OOM5+OOM6
```

```
      FUNFM=OOMA1+OOMA2+OOMA3+OOMA5+OOMA6
      IF (MI.EQ.1) GO TO 72
7     GO TO 73
   72 XFUNIM=FUNIM
   73 WRITE(6,1001)XFUNIM
      YF(1,I2)=XFUNIM
      YF(MI1,I2)=FUNFM
 1001 FORMAT (//10X,'INITIAL MINIMAZATION FUNCTION EQUALS ',E10.3)
      WRITE(6,1002) FUNFM
 1002 FORMAT (10X,'FINAL MINIMAZATION FUNCTION EQUALS ',E10.3)
      GO TO 99
   70 WRITE(6,1110) JC(1)
      GO TO 99
   99 CONTINUE
      N=N+1
      DO 100 J=1,K
      DM(N,J)=AUGP(M,J)
  100 CONTINUE
  101 CONTINUE
      WRITE(6,1040) I2
      DO 103 I=1,N
  103 WRITE(6,1030) (DM(I,J),J=1,K)
      N=N-MM
  102 CONTINUE
      WRITE(6,1050) N,K,MM
 1050 FORMAT(1H1,/////,35X,'TABLE  . EXPERIMENTAL DESIGN DATA FOR N=',I2
     1,', K=',I2,', M=',I2//)
      WRITE(6,1130)
 1130 FORMAT(10X,'--------------------------------------------------------
     1-------------------------------------------------------------')
      WRITE(6,1060)
 1060 FORMAT(10X,'TEST CASE ',5X,'1',9X, '2',9X, '3',9X, '4',9X, '5',9X,
     1'6',9X,'7',9X,'8',9X,'9',9X,'10')
```

```
      WRITE(6,1130)
      WRITE(6,1070)
 1070 FORMAT(/10X,' STEP NO. ',35X,'DETERMINANT OF THE (X X) MATRIX'/)
      IK=0
      MX=MM+1
      DO 104 I=1,MX
      WRITE(6,1140) IK,(YDET(I,J),J=1,10)
      IK=IK+1
  104 CONTINUE
 1140 FORMAT(14X,I2,4X,10F10.3)
      WRITE(6,1130)
      WRITE(6,1150)
 1150 FORMAT(/10X,' STEP NO. ',42X,'AVERAGE VARIANCE'/)
      IK=0
      DO 105 I=1,MX
      WRITE(6,1140) IK,(YV(I,J),J=1,10)
      IK=IK+1
  105 CONTINUE
      WRITE(6,1130)
      WRITE(6,1160)
 1160 FORMAT(/10X,' STEP NO. ',40X,'AVERAGE SQUARED BIAS'/)
      IK=0
      DO 106 I=1,MX
      WRITE(6,1140) IK,(YB(I,J),J=1,10)
      IK=IK+1
  106 CONTINUE
      WRITE(6,1130)
      WRITE(6,1170)
 1170 FORMAT(/10X,' STEP NO. ',37X,'MINIMUM MEAN SQUARE ERROR'/)
      IK=0
      DO 107 I=1,MX
```

```
      WRITE(6,1140) IK,(YCJ(I,J),J=1,10)
      IK=IK+1
  107 CONTINUE
      WRITE(6,1130)
      WRITE(6,1180)
 1180 FORMAT(/10X,' STEP NO. ',41X,'IMPROVEMENT RATIO'/)
      IK=1
      DO 108 I=1,MM
      WRITE(6,1140) IK,(YRI(I,J),J=1,10)
      IK=IK+1
  108 CONTINUE
      WRITE(6,1130)
      WRITE(6,1190)
 1190 FORMAT(/10X,' STEP NO. ',39X,'MINIMIZATION FUNCTION'/)
      IK=0
      DO 109 I=1,MX
      WRITE(6,1140) IK,(YF(I,J),J=1,10)
      IK=IK+1
  109 CONTINUE
      MH=MH+1
      IF(MH.LT.NH) GO TO 1
      STOP
      END
```

```
      SUBROUTINE XMA(DM,AUGP,XTX,XTXI,XATXA,XATXAI,DETX,DETXA,N,K,M,DA)
      DIMENSION DM(100,10) ,AUGP(10,10),XTX(11,11),XTXI(11,11)
      DIMENSION XATXA(11,11),XATXAI(11,11),DA(100,10) ,JC(20),V(2),U(2)
      DIMENSION X(100,11) ,XA(100,11) ,A(11,11),B(11,11)
      DO 10 I=1,N
      DO 10 J=1,K
      DA(I,J)=DM(I,J)
   10 CONTINUE
      N1=N
      DO 15 I=1,M
      N1=N1+1
      DO 15 J=1,K
      DA(N1,J)=AUGP(I,J)
   15 CONTINUE
      K1=K+1
      L1=N+M
      DO 20 I=1,N
      DO 20 J=1,K1
      IF (J.EQ.1) GO TO 17
      J1=J-1
      X(I,J)=DM(I,J1)
      GO TO 20
   17 X(I,J)=1.0
   20 CONTINUE
      DO 25 I=1,L1
      DO 25 J=1,K1
      IF (J.EQ.1) GO TO 22
      J2=J-1
      XA(I,J)=DA(I,J2)
      GO TO 25
   22 XA(I,J)=1.0
   25 CONTINUE
      CALL MXTMLT(X,N,K1,XTX,$50,100,11)
```

```
      CALL MXTMLT(XA,L1,K1,XATXA,$50,100,11)
      DO 35 I=1,K1
      DO 35 J=1,K1
      A(I,J)=XTX(I,J)
   35 B(I,J)=XATXA(I,J)
      V(1)=3
      CALL GJR(A,11,11,K1,K1,$55,JC,V)
      U(1)=3
      CALL GJR(B,11,11,K1,K1,$55,JC,U)
      DETX=V(1)*EXP(V(2))
      DETXA=U(1)*EXP(U(2))
      DO 40 I=1,K1
      DO 40 J=1,K1
      XTXI(I,J)=A(I,J)*N
      XATXAI(I,J)=B(I,J)*L1
   40 CONTINUE
      GO TO 60
   50 WRITE(6,100)
  100 FORMAT(1H1,'ERROR EXIT FROM MATHSTAT ROUTINE MXTMLT')
      GO TO 60
   55 WRITE(6,110) JC(1)
  110 FORMAT(1H1,10X,'ERROR RETURN FROM GJR-CONDITION-',I3)
   60 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE CKR(CJ,CJA,RI,XTX,XTXI,XATXA,XATXAI,N,K,M,DM,DA,MI,I2,Y
     1V,YB)
      DIMENSION YV(10,10),YB(10,10)
      DIMENSION XTX(11,11),XTXI(11,11),XATXA(11,11),XATXAI(11,11)
      DIMENSION OMM(10,10,10),OMMA(10,10,10),DM(100,10),DA(100,10)
      MI1=MI+1
      K1=K+1
      N1=N+M
      ALPHA=SQRT(N)/0.05
      ALPHAA=SQRT(N1)/0.05
      V=1.0
      VA=1.0
      DO 5 J=2,K1
      V=V+XTXI(J,J)/(K+2)
      VA=VA+XATXAI(J,J)/(K+2)
    5 CONTINUE
      IF (MI.EQ.1) GO TO 6
      GO TO 7
    6 XV=V
    7 WRITE(6,100) XV,VA
  100 FORMAT(//10X,'V=',E10.3,5X,'VA=',E10.3)
      YV(1,I2)=XV
      YV(MI1,I2)=VA
      DO 10 L1=1,K
      DO 10 L2=1,K
      DO 10 L3=1,K
      OMM(L1,L2,L3)=0
      OMMA(L1,L2,L3)=0
   10 CONTINUE
      DO 15 L1=1,K
      DO 15 L2=1,K
      DO 15 L3=1,K
      DO 15 I=1,N
```

```
      OMM(L1,L2,L3)=OMM(L1,L2,L3)+(DM(I,L1)*DM(I,L2)*DM(I,L3))
   15 CONTINUE
      DO 20 L1=1,K
      DO 20 L2=1,K
      DO 20 L3=1,K
      DO 20 I=1,N1
      OMMA(L1,L2,L3)=OMMA(L1,L2,L3)+(DA(I,L1)*DA(I,L2)*DA(I,L3))
   20 CONTINUE
      DO 21 L1=1,K
      DO 21 L2=1,K
      DO 21 L3=1,K
      OMM(L1,L2,L3)=OMM(L1,L2,L3)*(1.0/N)
      OMMA(L1,L2,L3)=OMMA(L1,L2,L3)*(1.0/N1)
   21 CONTINUE
      TF=0
      TFA=0
      DO 26 LG=2,K1
      FT=0
      FTA=0
      DO 25 LI=1,K
      DO 25 LJ=LI,K
      DO 25 LH=1,K
      LO=LH+1
      FT=FT+(ALPHA*XTXI(LG,LO)*OMM(LH,LI,LJ))
      FTA=FTA+(ALPHAA*XATXAI(LG,LO)*OMMA(LH,LI,LJ))
   25 CONTINUE
      TF=TF+(FT**2)
      TFA=TFA+(FTA**2)
   26 CONTINUE
      TF=TF*(1.0/(K+2))
      TFA=TFA*(1.0/(K+2))
      IF (MI.EQ.1) GO TO 27
      GO TO 22
   27 XTF=TF
```

```
   22 WRITE(6,101) XTF,TFA
  101 FORMAT(10X,'TF=',E10.3,5X,'TFA=',E10.3)
      DO 28 I=1,K1
      DO 28 J=1,K1
      XTX(I,J)=XTX(I,J)*(1.0/N)
      XATXA(I,J)=XATXA(I,J)*(1.0/N1)
   28 CONTINUE
      ST=0
      STA=0
      DO 30 LI=2,K1
      DO 30 LJ=LI,K1
      IF(LI.EQ.LJ) GO TO 29
      ST=ST+(ALPHA*(XTX(LI,LJ)))
      STA=STA+(ALPHAA*(XATXA(LI,LJ)))
      GO TO 30
   29 ST=ST+(ALPHA*(XTX(LI,LJ)-(1.0/(K+2))))
      STA=STA+(ALPHAA*(XATXA(LI,LJ)-(1.0/(K+2))))
   30 CONTINUE
      ST=ST**2
      STA=STA**2
      IF (MI.EQ.1) GO TO 31
      GO TO 32
   31 XST=ST
   32 WRITE(6,102) XST,STA
  102 FORMAT(10X,'ST=',E10.3,5X,'STA=',E10.3)
      AT=0
      ATA=0
      K2=K-1
      DO 35 LI=1,K2
      J=LI+1
      DO 35 LJ=J,K
      AT=AT+(ALPHA**2)
      ATA=ATA+(ALPHAA**2)
```

```
   35 CONTINUE
      TT=(2*(K+2)*K*(ALPHA**2)+(K+2)*AT-2*(K*ALPHA)**2)
     1/(((K+2)**2)*(K+4))
      TTA=(2*(K+2)*K*(ALPHAA**2)+(K+2)*ATA-2*(K*ALPHAA)**2)
     1/(((K+2)**2)*(K+4))
      IF (MI.EQ.1) GO TO 36
      GO TO 37
   36 XTT=TT
   37 WRITE(6,103) XTT,TTA
  103 FORMAT(10X,'TT=',E10.3,5X,'TTA=',E10.3)
      B=TF+ST+TT
      BA=TFA+STA+TTA
      IF (MI.EQ.1) GO TO 33
      GO TO 34
   33 XB=B
   34 WRITE(6,105) XB,BA
  105 FORMAT(10X,'B=',E10.3,5X,'BA=',E10.3)
      YB(1,I2)=XB
      YB(MI1,I2)=BA
      CJ=V+B
      IF (MI.EQ.1) GO TO 38
      GO TO 39
   38 XCJ=CJ
   39 CJA=VA+BA
      K2=K-1
      BETA=0
      DO 40 I=1,K2
      J1=I+1
      DO 40 J=J1,K
      BETA=BETA+1.0
   40 CONTINUE
      THETA=N*((K*1.0)+(0.5*BETA))
      THETAA=N1*((K*1.0)+(0.5*BETA))
```

```
      PHI=(K*1)**2/(THETA/N)
      PHIA=(K*1)**2/(THETAA/N1)
      CJB=(1+K)+THETA*((2*(K+2-PHI)/(((K+2)**2)*(K+4))))
      CJAB=(1+K)+THETAA*((2*(K+2-PHIA)/(((K+2)**2)*(K+4))))
      IF (MI.EQ.1) GO TO 41
      GO TO 42
   41 XCJB=CJB
   42 WRITE(6,104) XCJB,CJAB
  104 FORMAT(10X,'CJB=',E10.3,5X,'CJAB=',E10.3)
      RI=(CJA-CJAB)/(XCJ-XCJB)
      RETURN
      END
```

```
      SUBROUTINE RANMA (DM,N,K,LFY,YFL)
      DIMENSION DM(100,10),X(1000),XM(100)
      LFY=LFY+1
      IF (LFY.GT.1.0) GO TO 2
      X(1)=2516905
      GO TO 3
    2 X(1)=YFL
    3 CONTINUE
      CALL RANDU(X,1000)
      YFL=(X(1000)+X(999))*(1.E+7)
      DO 5 I=1,1000
      X(I)=X(I)*2.0-1.0
    5 CONTINUE
      DO 6 I=1,N
      XM(I)=0
    6 CONTINUE
      L1=0
      DO 15 I=1,N
      DO 15 J=1,K
      L1=L1+1
      DM(I,J)=X(L1)
      XM(I)=XM(I)+(DM(I,J)**2)
   15 CONTINUE
      DO 30 I=1,N
      L1=L1+1
      IF (XM(I).GT.1.05) GO TO 20
      GO TO 30
   20 DO 25 J=1,K
      DM(I,J)=(DM(I,J)/SQRT(XM(I)))*X(L1)
   25 CONTINUE
   30 CONTINUE
      RETURN
      END
```

BIBLIOGRAPHY

1. Box, G.E.P. and N.R. Draper: "A Basis for the Selection of a Response Surface Design," J. Amer. Statist. Assoc. Vol. 54, pp. 622-654, 1959.

2. Box, G.E.P. and N.R. Draper: "The Choice of a Second Order Rotatable Design," Tech. Rept. 10, University of Wisconsin, Dept. of Statistics, Madison, Wisconsin, July, 1962.

3. Box, G.E.P. and K.B. Wilson: "On Experimental Attainment of Optimum Conditions," J. Roy. Statist. Soc., B 13, 1, 1951.

4. Davies, O.L.: Design and Analysis of Industrial Experiments, New York, Hafner Publishing Company, 1954.

5. Dykstra, Otto Jr.: "The Orthogonolization of Undesigned Experiments," Technometrics, Vol. 8, No. 2, May, 1966, pp. 279-280.

6. Fisher, R.A., and F. Yates: Statistical Tables for Biological, Agricultural, and Medical Research, New York, Hafner Publishing Company, 1963.

7. Gaylor, D.W. and T.A. Merrill: "Augmenting Existing Data in Multiple Regression," Technometrics, Vol. 10, No. 1, pp. 73 - 81.

8. Hicks, C.R.: Fundamental Concepts in the Design of Experiments, Holt, Reinhart, and Winston, 1964.

9. Kempthorne, O.: The Design and Analysis of Experiments, New York, WIley, 1952.

10. Kennard, R.W. and L.A. Stone: "Computer Aided Design of Experiments," Technometrics, Vol. 11, No. 1, Feb., 1969, pp. 137 - 148.

11. Mitchell, T.J.: "Computer-Aided Design of Experiments: Augmenting Existing Data," Unpublished Paper Presented at SRER Summer Conference in Statistics, Mountain Lake, Virginia, June 14, 1971.

BIBLIOGRAPHY (Concluded)

12. Myers, Raymond H.: Response Surface Methodology, Allyn and Bacon, Inc., 1971, pp. 27 - 29, 110 - 114, 240 - 142, 196 - 211.

13. Plackett, R.L.: "Some Theorems in Least Squares," Biometrika, 37, 1950, pp. 149 - 157.

14. Sperry Rand Corporation, Large Scale Systems Math-Pack, Remington Rand UNIVAC, RANDU Sec. 14.2, pp. 4 - 7.